

## Supporting Information

### A Theoretical Study of the Kinetics of the Gas-Phase Reaction between Phenyl and Amino Radicals

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#### Calculate the rate constants with the VTST

For the barrierless transition state processes,  $C_6H_5 + NH_2 \rightarrow C_6H_5NH_2$ , the VRC-TST method was employed to calculate rate constants based on the evaluation of the maximum free energy of activation ( $\Delta G^\ddagger$ ) at each temperature along the reaction path. The potential energy surface for the dissociation of  $C_6H_5NH_2$  was scanned at the B3LYP/6-311++G(3df,2p) level of theory. In which, the C-N bond distance of  $C_6H_5NH_2$  was changed from 4.0 Å to its equilibrium value, 1.395 with an interval of 0.1 Å. The geometric structures with the fixed bond distance of C-N were optimized at the same level above to obtain the rotational and vibrational parameters. The B3LYP calculated energy at each point along the reaction path was employed to evaluate the Morse potential energy function and then scaled to match the dissociation energy estimated at the CCSD(T) level. The Morse potential energy  $V(R)$  utilized to describe the minimum potential energy along the reaction path is presented as follows

$$V(R) = D_e \{1 - \exp[-\beta(R - R_e)]\}^2$$

where  $D_e$  is the bonding energy excluding zero-point vibrational energy (ZPVE) for an association reaction,  $R$  is the bond distance between two bonding atoms (i.e., in the present work C-N),  $R_e$  is the equilibrium value of  $R$  at the stable intermediate structure.

The predicted moments of inertia, the vibrational frequencies, and the dissociation energy as a function of R were used to find  $\Delta G^{\ddagger}_{\max}$  at each temperature in the range of 300 - 2000 K. All the molecular parameters corresponding to the structure with a  $\Delta G^{\ddagger}_{\max}$  for each temperature were then used for the RRKM calculation.

**Table S1.** Frequencies of reactants, intermediates, transition states and products of the  $C_6H_5 + NH_2$  reaction at the B3LYP/6-311++G(3df,2p) method.

C <sub>6</sub> H <sub>5</sub>	401.11	991.22	1464.31
	427.65	1000.83	1472.59
	602.41	1017.04	1570.10
	620.84	1052.31	1627.01
	667.49	1072.94	3154.12
	724.33	1177.05	3159.67
	817.45	1177.41	3173.33
	899.04	1303.34	3175.09
	969.56	1326.02	3185.97
NH <sub>2</sub>	1530.82	3363.96	3452.32
IS1	219.40	889.61	1501.16
	292.73	973.88	1531.71
	383.30	983.66	1623.73
	417.60	990.86	1642.39
	502.26	1047.34	1659.08
	535.38	1061.82	3150.32
	570.08	1133.52	3153.08
	633.86	1179.88	3168.64
	697.57	1201.25	3174.07
	762.63	1292.30	3192.28
	824.68	1343.59	3568.99
829.39	1369.81	3665.82	
IS2	121.67	952.73	1442.13
	321.85	965.83	1445.25
	376.07	987.99	1634.74
	433.97	1015.49	1661.74
	510.11	1027.94	1717.86
	570.31	1118.98	2975.77
	592.07	1189.65	2978.92
	735.75	1207.93	3139.08
	781.15	1208.22	3150.11
	835.75	1355.91	3160.43
	884.01	1382.98	3183.32

	913.22	1421.82	3438.23
IS3	108.77	875.33	1401.79
	148.04	926.17	1432.61
	358.27	957.30	1528.76
	372.89	983.70	1623.99
	406.26	1013.10	1626.80
	438.19	1078.70	2928.14
	510.66	1124.83	2974.50
	570.57	1173.00	3122.48
	593.73	1191.73	3155.72
	689.00	1276.98	3176.15
	768.32	1307.85	3556.45
	817.29	1320.36	3670.89
IS4	122.20	851.81	1380.19
	253.85	904.34	1428.65
	328.20	957.17	1599.95
	363.24	977.64	1655.56
	442.55	996.67	1828.70
	506.71	1095.84	2982.92
	538.93	1137.15	3146.25
	580.15	1149.71	3148.15
	717.41	1169.62	3155.09
	759.81	1247.68	3171.26
	789.93	1277.55	3491.78
819.20	1348.31	3572.30	
IS5	124.34	896.44	1430.35
	252.16	919.02	1461.19
	268.89	947.75	1597.52
	397.98	961.22	1636.73
	413.70	991.60	1684.79
	474.63	1046.24	2993.12
	544.97	1150.51	3046.26
	582.29	1173.91	3103.46
	630.85	1283.98	3150.41
	702.16	1300.53	3179.77
	801.54	1380.68	3568.90
859.53	1398.68	3706.79	
IS6	90.51	848.27	1366.97
	206.43	922.79	1413.76
	282.84	962.43	1509.26
	345.30	974.24	1579.22
	389.29	1016.13	1628.99
	447.29	1064.49	2756.03
	539.08	1112.26	3134.51
	651.33	1151.56	3144.74
	712.16	1180.93	3155.83
	774.77	1226.37	3173.46

	802.34	1269.70	3482.26
	836.46	1315.92	3571.10
IS7	163.19	845.82	1415.19
	297.89	881.71	1445.73
	339.92	923.79	1580.74
	390.70	987.16	1656.72
	423.37	1030.67	1764.00
	438.39	1106.07	2984.10
	470.00	1157.97	3041.37
	552.31	1181.33	3134.59
	614.82	1261.75	3142.44
	671.95	1301.96	3148.23
	750.71	1312.20	3583.91
	800.06	1382.40	3689.81
IS8	74.75	885.51	1401.34
	191.08	930.56	1414.96
	260.26	941.82	1538.54
	372.01	1012.56	1606.15
	391.61	1030.90	1658.72
	444.32	1083.74	2945.52
	520.02	1131.75	3025.20
	547.81	1179.53	3104.05
	590.39	1254.80	3121.43
	785.91	1270.96	3158.96
	791.02	1348.44	3584.49
	807.73	1363.74	3703.05
IS9	199.03	821.26	1411.06
	210.16	871.81	1454.44
	311.63	935.05	1626.11
	371.29	949.02	1656.30
	387.94	998.34	1812.41
	487.02	1125.52	2964.08
	524.58	1154.25	3029.87
	575.08	1168.24	3139.50
	640.72	1225.09	3146.28
	724.28	1272.40	3156.40
	754.67	1302.49	3556.43
	764.03	1378.02	3651.84
IS10	77.57	879.63	1418.99
	230.00	889.31	1464.33
	314.79	951.52	1494.42
	319.37	973.57	1654.70
	386.99	989.77	1665.44
	513.08	1055.90	2965.07
	528.07	1164.44	2967.93
	580.71	1177.87	3045.24
	596.84	1268.32	3123.96

	795.85	1314.36	3151.94
	804.41	1344.50	3586.94
	828.12	1367.05	3703.77
IS11	186.39	950.75	1464.76
	205.50	985.06	1577.66
	325.81	1003.51	1592.31
	409.44	1020.73	1625.91
	454.47	1030.47	1630.69
	499.84	1052.28	3107.00
	615.95	1139.78	3125.80
	701.42	1174.43	3142.51
	737.65	1277.81	3177.58
	740.08	1330.47	3196.57
	876.24	1362.17	3415.16
	938.78	1439.86	3475.53
IS12	107.73	957.06	1444.98
	186.34	974.29	1539.59
	313.05	981.64	1595.75
	375.84	1008.72	1641.91
	421.48	1010.66	1659.02
	499.20	1083.99	2959.89
	595.80	1113.44	3080.74
	687.34	1182.09	3125.73
	729.57	1287.06	3155.54
	733.49	1328.68	3370.68
	825.63	1412.11	3444.85
	896.81	1420.53	3458.96
IS13	64.06	951.83	1431.18
	272.37	967.08	1448.03
	438.63	993.86	1609.60
	449.16	1003.68	1652.93
	488.48	1008.85	1698.60
	552.90	1119.42	2980.31
	589.99	1194.73	3055.81
	707.70	1199.59	3147.34
	757.51	1204.37	3156.50
	793.53	1334.11	3167.55
	914.20	1367.73	3182.14
	939.13	1409.58	3437.17
IS14	170.13	901.58	1410.57
	245.30	924.50	1477.10
	268.01	937.29	1484.81
	360.67	970.79	1606.14
	440.25	999.90	1642.78
	514.93	1037.72	3149.30
	620.16	1073.11	3150.49
	620.24	1141.37	3179.52

	652.18	1157.64	3182.37
	779.45	1209.06	3393.72
	792.49	1286.79	3486.42
	817.08	1321.98	3493.37
IS16	75.63	864.13	1379.45
	118.57	888.63	1444.72
	215.68	970.90	1521.31
	295.32	996.87	1640.71
	378.00	1018.11	1665.90
	499.28	1116.25	2945.46
	522.44	1126.96	2951.17
	607.67	1172.98	3102.24
	630.81	1230.34	3122.01
	711.02	1247.48	3132.32
	773.34	1284.40	3553.48
	838.93	1333.13	3648.60
IS18	97.75	919.11	1416.50
	154.27	932.22	1453.40
	259.61	952.33	1491.11
	312.03	997.65	1614.70
	381.90	1020.80	1655.79
	463.86	1065.29	2982.66
	494.83	1196.31	3010.73
	565.33	1202.34	3050.99
	596.71	1298.25	3110.26
	732.78	1317.69	3135.50
	781.67	1394.27	3587.42
	890.93	1409.61	3703.29
IS19	153.71	901.20	1415.24
	225.15	933.45	1438.44
	360.30	936.64	1546.22
	386.91	1004.68	1587.56
	421.30	1017.98	1628.96
	439.05	1121.76	2952.20
	526.94	1148.12	2958.95
	570.43	1157.93	3115.87
	577.87	1237.55	3121.25
	721.10	1291.67	3148.36
	788.16	1353.80	3549.98
	805.02	1383.46	3665.61
IS20	122.74	871.68	1432.95
	296.52	910.05	1453.27
	312.92	949.16	1601.58
	327.75	979.20	1630.84
	410.48	1009.56	1676.01
	483.38	1051.92	2955.63
	557.79	1155.63	3001.30

	589.98	1183.99	3091.08
	637.18	1302.72	3127.57
	756.56	1323.66	3162.56
	783.11	1356.20	3561.32
	805.97	1410.90	3700.16
T1/2	-1718.29	927.18	1373.11
	316.91	948.42	1434.17
	398.32	960.18	1443.16
	441.21	978.84	1484.63
	505.71	1007.13	1497.56
	563.48	1052.76	1584.77
	628.18	1107.50	3165.90
	637.77	1145.79	3174.08
	668.26	1157.33	3183.63
	755.25	1264.88	3203.60
	829.24	1315.50	3205.25
	901.74	1332.97	3418.24
T1/3	-388.36	866.88	1405.09
	110.05	918.29	1440.95
	367.75	934.82	1542.90
	382.75	995.89	1623.61
	401.92	999.88	1632.03
	464.79	1035.56	2603.97
	512.01	1124.52	3095.04
	540.49	1181.88	3123.17
	604.87	1200.74	3163.83
	655.80	1245.55	3183.15
	718.60	1298.12	3560.86
	820.72	1361.77	3677.92
T1/4	-1421.84	808.38	1351.62
	232.35	841.80	1423.58
	315.20	929.08	1483.46
	338.82	943.07	1594.02
	380.92	1023.81	1643.85
	507.58	1053.11	1770.58
	547.39	1075.61	3122.95
	570.28	1134.17	3161.44
	645.94	1219.23	3178.05
	689.61	1255.87	3195.00
	718.93	1309.07	3543.65
	792.61	1332.26	3641.33
T1/6	-264.12	901.96	1413.48
	119.19	934.58	1442.19
	248.02	1001.61	1523.37
	356.17	1011.67	1630.22
	388.59	1036.98	1666.60
	512.60	1071.80	2681.53

	557.47	1090.77	3117.55
	601.17	1164.49	3139.49
	647.55	1198.94	3167.50
	746.15	1203.39	3185.96
	848.78	1249.50	3502.64
	890.20	1276.61	3568.13
T1P8	-1512.65	897.83	1319.95
	265.06	922.00	1506.63
	318.05	930.08	1530.91
	349.47	952.01	1533.23
	404.41	955.32	1570.84
	428.14	996.79	1803.28
	545.05	1010.58	3147.08
	699.69	1045.71	3148.24
	725.73	1139.71	3175.39
	774.13	1142.94	3178.63
	792.62	1219.03	3518.36
	833.42	1291.30	3616.45
T1/7	-1577.88	827.01	1363.26
	228.01	906.77	1437.07
	325.98	916.26	1506.66
	363.71	948.53	1582.22
	398.03	1050.68	1649.07
	447.98	1055.56	1764.47
	498.65	1071.52	3043.20
	536.18	1121.56	3123.88
	589.22	1232.35	3148.40
	648.26	1259.25	3166.12
	716.95	1273.51	3562.28
	785.87	1330.22	3667.05
T1/8	-1034.40	815.18	1421.69
	164.08	900.74	1464.35
	358.40	985.70	1545.09
	381.41	1010.91	1624.29
	390.60	1019.72	1656.92
	410.92	1039.51	2218.03
	454.50	1112.88	3075.64
	530.64	1190.70	3126.58
	613.42	1207.63	3143.10
	680.89	1247.51	3158.98
	783.31	1314.01	3582.87
	807.49	1371.02	3689.88



T1/9	-1491.48	811.76	1346.57
	229.22	835.62	1435.08
	323.03	889.04	1497.32
	348.98	988.56	1592.20
	400.64	1051.37	1655.34
	459.48	1065.72	1756.34
	503.15	1082.24	3109.45
	565.21	1118.08	3134.65
	593.45	1219.77	3155.59
	641.08	1233.37	3161.50
	697.72	1269.05	3584.77
	784.70	1312.37	3681.69
T1/10	-1088.03	846.75	1425.78
	160.61	888.84	1483.67
	337.44	967.47	1518.47
	348.74	982.26	1639.91
	384.67	1000.48	1657.47
	442.29	1042.50	2185.36
	509.07	1110.65	3091.01
	532.22	1188.84	3108.57
	606.56	1228.34	3142.10
	656.47	1279.87	3162.78
	758.28	1311.89	3589.57
	812.90	1374.95	3698.74
T1/11	1288.0171	199.8175	351.6162
	425.51120	454.7764	492.9765
	596.08000	637.6614	711.1373
	749.47660	818.6959	882.6828
	947.99080	1002.8476	1003.2515
	1037.7133	1048.7871	1099.3419
	1103.3918	1147.5327	1178.1568
	1283.2238	1320.7875	1414.8575
	1451.4256	1468.5229	1580.2717
	1589.4789	1604.6653	1966.6625
	3128.8995	3148.9076	3155.5288
	3178.5280	3423.3497	3510.6805
T1/13	-2043.17	875.28	1402.48
	206.88	956.64	1457.04
	360.56	993.24	1522.72
	448.17	996.20	1539.56
	506.80	1002.03	1618.61
	562.10	1045.05	1776.81
	611.45	1119.29	3071.64
	638.62	1168.95	3152.93
	652.78	1181.55	3160.91
	757.42	1200.87	3175.83
	786.38	1314.15	3186.33

	822.37	1372.23	3435.17
T1/16	-410.17 190.52 242.05 312.68 380.80 474.49 512.02 566.11 623.50 646.48 776.03 820.38	863.01 884.10 928.54 998.29 1019.61 1038.20 1124.25 1178.97 1228.17 1247.64 1287.59 1367.18	1397.38 1465.70 1536.13 1641.16 1663.21 2566.82 3094.50 3108.79 3129.48 3145.40 3563.58 3661.80
T1/18	-976.36 190.71 255.29 354.84 372.12 437.74 569.47 625.49 643.49 689.29 739.98 747.69	810.33 874.62 924.98 955.76 991.99 1049.82 1080.07 1103.05 1147.97 1219.45 1225.37 1326.55	1350.45 1396.41 1567.60 1631.73 1672.51 1939.01 3092.65 3197.76 3219.88 3224.46 3533.29 3628.66
T1/19	-802.57 185.42 315.05 346.22 441.44 491.05 521.54 587.27 641.99 702.99 727.29 789.02	839.37 858.70 887.15 901.86 980.64 1047.08 1085.67 1094.17 1199.04 1247.17 1265.00 1317.93	1358.73 1380.59 1565.73 1630.39 1670.49 2071.20 3093.73 3194.88 3209.79 3221.81 3554.48 3650.54
T1/20	-1605.02 216.82 298.31	848.94 893.63 924.77	1360.99 1441.08 1487.06

	362.30	956.47	1606.04
	375.63	1013.93	1649.06
	499.75	1043.03	1737.75
	504.37	1064.95	3089.12
	544.11	1146.94	3108.78
	581.01	1225.42	3152.94
	631.26	1248.51	3172.11
	735.72	1303.34	3563.87
	786.13	1328.00	3677.02
T1P1	-2063.38	803.50	1353.25
	261.96	861.91	1354.69
	320.39	876.55	1402.98
	457.96	947.49	1496.51
	516.11	978.67	1560.26
	526.04	1006.03	1587.24
	572.68	1083.36	1649.14
	581.95	1115.83	3155.57
	637.08	1148.91	3169.79
	674.92	1245.34	3179.74
	739.82	1275.88	3197.21
	785.44	1322.42	3437.05
T1P2	-1876.21	800.36	1347.58
	198.11	820.58	1394.21
	278.60	884.39	1464.61
	375.86	909.86	1499.50
	424.19	967.10	1540.28
	489.80	1029.97	1687.52
	547.71	1036.24	3166.51
	601.55	1074.68	3168.52
	657.10	1086.27	3183.14
	676.63	1109.94	3233.45
	725.68	1243.14	3476.73
	767.76	1276.70	3595.68
T1/11	-1288.02	947.99	1451.43
	199.82	1002.85	1468.52
	351.62	1003.25	1580.27
	425.51	1037.71	1589.48
	454.78	1048.79	1604.67
	492.98	1099.34	1966.66
	596.08	1103.39	3128.90
	637.66	1147.53	3148.91
	711.14	1178.16	3155.53
	749.48	1283.22	3178.53
	818.70	1320.79	3423.35
	882.68	1414.86	3510.68

T2P6	-246.95	770.29	1372.11
	140.69	783.87	1407.43
	207.15	830.56	1458.78
	225.13	876.73	1493.71
	337.74	892.60	1533.43
	410.37	960.44	1591.56
	469.38	972.08	3144.81
	513.65	1012.49	3155.69
	543.00	1096.34	3162.03
	619.58	1174.53	3180.96
	640.28	1187.28	3441.00
	734.74	1287.44	3844.11
T3P4	-1143.60	766.12	1357.66
	176.94	773.98	1440.59
	362.39	856.58	1496.01
	378.98	878.18	1557.85
	397.39	945.46	1632.98
	441.17	960.84	1687.65
	486.27	1028.11	3134.03
	526.06	1098.75	3176.75
	586.79	1152.80	3196.13
	620.58	1176.38	3254.55
	665.99	1180.08	3571.46
	726.45	1299.58	3684.46
T4P2	-576.20	790.57	1402.67
	74.20	850.19	1468.73
	147.91	868.01	1490.55
	177.80	916.29	1536.04
	253.64	969.46	1660.68
	398.56	998.22	2873.03
	454.21	1048.04	3148.94
	562.56	1090.87	3163.07
	597.42	1164.72	3176.91
	631.79	1190.68	3189.59
	649.41	1282.87	3413.19
	727.24	1322.02	3504.00
T5P12	-1210.75	776.46	1381.20
	176.74	826.63	1444.50
	316.18	871.66	1458.61
	348.53	901.67	1563.37
	366.36	931.77	1618.76
	463.61	964.73	1661.64
	504.29	995.68	2497.86
	532.91	1077.97	3118.98
	552.79	1149.36	3156.25
	579.34	1208.14	3198.04
	636.76	1263.55	3541.37

	677.86	1286.88	3653.76
T6/5	-997.44 184.82 341.00 363.13 426.61 482.53 538.10 547.21 612.51 639.92 761.26 794.84	916.17 947.95 958.14 1009.91 1020.00 1041.87 1080.48 1135.83 1182.05 1270.31 1300.40 1337.59	1424.55 1438.15 1546.20 1583.13 1619.07 1993.61 3102.94 3137.33 3148.15 3192.98 3552.67 3671.85
T7P7	-1809.41 231.17 239.73 342.81 415.46 463.30 500.57 610.25 646.67 689.07 750.38 808.87	828.36 859.52 929.62 942.95 1034.16 1076.25 1089.41 1119.26 1152.46 1291.66 1336.88 1345.24	1397.40 1412.51 1540.06 1581.15 1650.45 1718.87 2983.80 3116.85 3126.33 3131.91 3459.79 3573.30
T7P11	-1108.37 226.49 278.85 338.42 385.89 418.25 428.43 539.60 558.06 574.17 594.06 703.59	750.75 798.00 869.14 880.61 929.50 971.89 1080.27 1094.00 1131.01 1163.76 1277.96 1317.41	1329.06 1430.79 1436.82 1545.92 1623.06 1650.27 2331.24 3126.88 3143.06 3157.51 3544.86 3650.06
T8P4	-1227.13 167.26 222.78 349.90 371.27 422.64 527.66 532.80	790.30 821.00 841.83 887.42 952.82 991.60 1043.66 1071.18	1360.05 1455.78 1479.18 1552.64 1654.11 1692.32 3126.24 3144.31

	563.06	1095.51	3166.19
	613.86	1160.48	3172.25
	649.43	1213.40	3561.65
	781.81	1321.43	3655.26
T9P3	-1214.65	754.38	1365.77
	196.42	806.98	1446.52
	275.87	831.09	1499.58
	318.87	850.82	1542.78
	370.47	969.26	1637.23
	478.51	989.67	1656.24
	497.94	1047.29	2339.05
	520.65	1087.42	3111.74
	523.42	1118.05	3161.26
	570.86	1193.00	3184.68
	609.92	1268.34	3580.39
	637.93	1300.31	3678.36
T10P10	-1130.58	766.89	1370.99
	197.20	796.73	1419.68
	341.79	805.43	1494.56
	387.40	889.63	1562.37
	397.10	932.33	1654.46
	416.50	952.68	1683.04
	452.94	1009.95	3085.67
	489.13	1049.06	3158.25
	536.85	1076.85	3173.76
	584.87	1148.14	3297.10
	662.90	1288.35	3579.95
	755.35	1289.66	3681.93
T11P5	-131.96	874.95	1485.76
	16.33	894.48	1509.13
	107.88	930.12	1636.37
	151.28	985.09	1652.53
	394.26	1015.21	1833.47
	422.02	1038.68	3132.68
	432.20	1065.03	3154.60
	491.01	1115.73	3171.00
	540.11	1161.39	3191.08
	635.27	1264.93	3466.07
	647.44	1334.64	3601.54
	746.18	1430.56	3618.20
T12P2	-273.36	816.92	1441.86
	71.44	864.82	1511.35
	103.27	891.72	1643.41
	190.68	973.47	1647.79
	364.12	986.93	1666.39
	452.42	1048.33	3102.15
	471.37	1089.02	3104.25

	522.60	1104.02	3122.49
	523.14	1155.47	3189.97
	602.95	1274.42	3467.33
	632.13	1309.32	3604.68
	771.25	1401.35	3612.88
T13P1	-478.03	814.84	1387.74
	152.22	864.04	1421.02
	191.09	914.84	1474.33
	330.64	960.89	1530.79
	390.47	989.74	1539.26
	424.27	1000.32	1617.59
	478.15	1026.12	2482.03
	545.23	1087.24	3160.35
	605.94	1148.84	3175.96
	658.84	1165.27	3187.12
	763.93	1188.52	3194.21
	798.94	1339.37	3433.17
T13P9	-293.64	739.71	1347.99
	112.02	779.10	1381.13
	178.18	818.21	1405.56
	213.36	848.38	1513.84
	330.34	897.14	1533.03
	394.60	916.45	1595.02
	447.18	973.61	3143.95
	496.28	1021.82	3152.88
	526.79	1061.40	3164.39
	552.15	1162.52	3177.93
	614.67	1181.19	3459.04
	680.92	1281.10	3837.71
T14P8	-389.37	802.75	1371.28
	93.50	854.15	1425.46
	152.14	890.92	1444.85
	174.83	904.91	1633.56
	289.13	953.28	1635.63
	378.33	978.07	3136.86
	480.58	1006.60	3138.07
	512.51	1052.91	3189.78
	566.43	1144.12	3192.06
	672.25	1178.49	3473.38
	697.41	1257.30	3617.34
	707.42	1291.11	3623.68
T16P10	-1173.28	771.42	1369.53
	223.23	816.43	1411.71
	251.59	828.62	1484.94
	312.50	860.37	1594.23
	377.78	961.50	1656.73
	432.65	984.76	1677.74

	502.56	1039.56	3112.49
	504.18	1095.66	3134.73
	589.91	1155.37	3157.92
	662.01	1169.92	3218.20
	667.10	1240.49	3562.27
	747.40	1299.24	3656.65
T18P2	-1834.28	902.73	1415.98
	173.94	920.79	1460.29
	238.99	972.88	1495.75
	308.83	985.78	1548.42
	365.47	1010.63	1570.95
	428.66	1066.79	1676.03
	542.92	1090.69	3073.54
	597.43	1120.97	3084.02
	680.16	1177.81	3099.27
	705.50	1238.04	3141.23
	784.29	1293.75	3468.34
	832.73	1330.80	3580.97
T18P3	-649.92	693.80	1380.09
	109.43	770.83	1426.95
	169.51	818.70	1483.94
	239.18	845.73	1555.86
	332.36	888.57	1648.76
	354.68	988.68	1653.29
	388.74	1039.90	1809.24
	433.38	1053.50	3019.10
	475.58	1109.19	3099.14
	498.59	1216.85	3151.71
	529.49	1263.48	3572.06
	607.70	1296.11	3679.80
T19P15	-897.99	690.33	1335.48
	182.54	763.76	1423.82
	264.42	808.40	1443.08
	313.81	857.70	1482.89
	388.37	912.65	1606.60
	396.42	1002.98	1633.47
	436.65	1036.82	2162.52
	462.35	1060.69	3136.36
	528.88	1117.02	3176.02
	580.98	1178.40	3214.78
	619.79	1243.09	3579.70
	643.43	1273.79	3697.46
T20P11	-1007.64	768.65	1368.26
	160.31	815.31	1410.00
	360.20	852.61	1456.98
	379.20	904.60	1557.26
	415.52	933.74	1618.24



	416.99	943.18	1637.73
	460.06	1007.17	2480.60
	482.79	1062.24	3125.17
	514.28	1148.81	3138.43
	526.70	1202.24	3198.24
	616.54	1293.87	3564.13
	701.07	1310.73	3681.37
PR1	156.94	809.53	1377.48
	364.64	869.36	1407.05
	401.05	914.01	1565.23
	444.20	968.87	1608.72
	510.95	1001.16	1805.11
	581.52	1053.09	3152.44
	613.88	1132.84	3161.39
	745.39	1174.18	3174.60
	766.54	1254.05	3184.07
	794.13	1315.86	3439.36
PR2	316.62	835.53	1385.29
	362.72	909.28	1420.65
	570.42	979.90	1558.64
	585.05	1076.73	1831.15
	617.44	1079.11	3154.93
	776.47	1088.40	3163.97
	821.63	1166.18	3203.80
	822.66	1304.90	3208.16
PR3	191.53	737.98	1375.97
	336.55	761.91	1510.91
	369.86	795.14	1574.55
	409.08	944.42	1655.57
	486.12	957.48	1830.19
	501.21	1028.82	3187.31
	566.79	1086.03	3189.00
	613.82	1148.18	3191.76
	646.52	1279.70	3604.16
	683.95	1282.33	3712.44
PR4	206.81	798.56	1455.46
	336.86	849.76	1468.21
	381.42	918.94	1525.78
	440.18	937.13	1650.24
	442.52	1003.57	2018.24
	492.12	1075.49	3145.37
	557.64	1158.99	3163.83
	561.90	1186.14	3222.98
	626.46	1292.23	3581.81
		735.86	1330.06

PR5	396.01	928.84	1424.24
	423.83	969.76	1463.54
	450.59	998.49	1483.01
	595.01	1075.15	2013.39
	627.74	1108.27	3156.98
	753.75	1161.94	3172.77
	844.73	1275.65	3196.82
	873.38	1306.10	3200.28
PR6	184.25	878.02	1402.96
	312.62	891.33	1451.58
	405.41	955.99	1482.66
	468.27	969.42	1514.31
	523.47	1016.34	1586.88
	530.84	1095.37	3141.37
	666.95	1173.70	3150.84
	769.21	1184.53	3157.98
	780.49	1284.86	3178.94
825.07	1371.25	3440.23	
PR7	307.34	788.96	1302.01
	456.14	848.94	1402.03
	475.44	902.44	1479.90
	491.35	943.24	1703.80
	548.10	1078.05	3197.92
	668.49	1090.60	3201.70
	722.18	1165.10	3219.05
	742.01	1238.29	3219.45
PR8	221.85	854.53	1308.35
	260.60	909.35	1355.13
	524.84	915.64	1582.46
	742.15	942.77	1632.36
	794.23	995.53	3136.75
	810.58	1124.92	3138.41
	821.17	1224.55	3155.22
	832.43	1283.86	3160.40
PR9	160.34	889.92	1392.43
	302.29	920.65	1404.19
	417.48	947.59	1500.76
	430.87	986.61	1534.58
	451.19	1019.47	1600.19
	535.88	1088.68	3138.16
	686.01	1164.03	3152.86
	759.29	1179.25	3169.96
	786.71	1295.03	3186.11
	828.33	1374.12	3433.20
PR10	242.55	821.78	1416.96
	261.71	841.71	1470.33
	384.84	924.38	1522.61

	394.65	937.08	1657.23
	412.44	1068.87	2013.43
	437.85	1088.85	3154.56
	563.53	1142.01	3172.29
	601.68	1251.77	3191.30
	656.60	1289.85	3569.09
	705.94	1325.88	3663.99
PR11	138.28	775.53	1408.99
	199.58	832.71	1441.87
	269.96	859.54	1572.23
	322.84	936.86	1650.23
	374.72	997.70	1818.17
	532.82	1084.83	3133.45
	561.39	1103.97	3168.80
	615.00	1199.34	3187.01
	670.32	1301.47	3549.96
	716.55	1318.77	3644.12
PR12	163.75	793.03	1391.90
	310.33	805.21	1431.64
	382.07	909.82	1570.12
	414.35	920.05	1622.60
	480.51	947.77	1943.26
	529.89	1075.52	3168.46
	572.76	1080.92	3210.31
	617.19	1217.95	3214.93
	631.86	1268.25	3573.86
	765.69	1307.12	3688.22
PR15	188.93	697.07	1337.05
	315.49	761.28	1453.77
	368.61	804.79	1533.40
	393.59	826.02	1640.08
	441.83	886.20	1725.45
	462.63	1016.58	3161.06
	562.68	1136.00	3167.50
	589.71	1139.05	3204.54
	667.94	1239.98	3583.46
	689.09	1282.26	3700.35

**Table S2.** Optimized coordinates of reactants, intermediates, transition states and products of the  $C_6H_5 + NH_2$  reaction at the B3LYP/6-311++G(3df,2p) level of theory.

$C_6H_5$	C,0,-1.626850123,1.1995022696,0.0059736753 C,0,-0.2276986595,1.1857469769,-0.0137437076 C,0,0.3934452705,2.4071742905,-0.0224360666 C,0,-0.2263432753,3.6292891918,-0.0136412981 C,0,-1.6255091383,3.6170844173,0.0060749969
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	C,0,-2.3158948367,2.4086755074,0.0157437511 H,0,-2.1707667147,0.2630739519,0.0135919266 H,0,0.3210706558,0.2532291414,-0.0215232797 H,0,0.3234602005,4.5611983197,-0.0213427314 H,0,-2.1683865598,4.5541149161,0.0137717654 H,0,-3.3975243807,2.409274827,0.0309859936
NH <sub>2</sub>	N,0,0.4997510918,1.4586319593,-0.0282739994 H,0,0.8677012401,0.5007321192,0.0195639089 H,0,0.8677182128,1.8961460369,0.8252068208
IS1	C,0,3.8777520441,0.5617233493,0.0150452085 C,0,3.9352371373,-0.7079713334,-0.5418555543 C,0,2.8371747517,-1.5601679196,-0.4875657891 C,0,1.6749262034,-1.1180841169,0.1358589586 C,0,1.6069215177,0.1497012254,0.6959040385 C,0,2.7096603316,1.0093831214,0.6421379012 H,0,4.7421276889,1.2130912148,-0.0298993125 H,0,4.8485849074,-1.0326324487,-1.0231828119 H,0,0.8092557356,-1.7655302804,0.1879502172 H,0,2.8859243478,-2.5482267829,-0.9228865287 N,0,2.6653008791,2.26254335,1.2524839688 H,0,3.3237774433,2.9415773374,0.9058434011 H,0,1.746298031,2.6553471812,1.3788872234 H,0,0.697302731,0.4793462025,1.1829293291
IS2	C,0,0.8425140561,0.002257148,0.1387374295 C,0,2.2955057345,0.309969182,-0.0238891687 C,0,2.6037887499,1.7726115134,-0.0201881828 C,0,1.665871043,2.71219312,0.1159090351 C,0,0.2456007079,2.3816288606,0.2740591813 C,0,-0.0875524588,0.9498767145,0.2741301983 H,0,0.5563456279,-1.0433144731,0.1438364193 H,0,2.8691501561,-0.1933063612,0.7662352577 H,0,3.6433146941,2.0569794712,-0.1347817413 H,0,1.912455181,3.7657244551,0.1156872666 H,0,-1.132872311,0.6860276405,0.3899666983 N,0,-0.6041548266,3.335250559,0.4001624037 H,0,-1.5513253167,2.968680292,0.5016367576 H,0,2.6669456732,-0.1463410212,-0.9515012477
IS3	C,0,1.116309884,-1.15318924,-0.4047714061 C,0,1.836984827,0.0711737651,0.0236798357 C,0,1.1242985775,1.2088272331,0.1657614317 C,0,-0.2949574891,1.1937674001,0.0265048245 C,0,-1.0097718197,0.003622586,-0.0600746655 C,0,-0.3545252174,-1.155349636,-0.5181741451 H,0,1.3381260012,-1.982087825,0.2950924824 H,0,2.9002371534,0.0335491663,0.2256273461 H,0,1.6085659698,2.1475360832,0.4031366791 H,0,-0.8222714392,2.1433525949,0.0148541985

	N,0,-2.3918081751,-0.0177900298,0.0817141121 H,0,1.5473867973,-1.5548030323,-1.3329109922 H,0,-2.8021115497,0.5831254958,0.7777039925 H,0,-2.7905595199,-0.9431355715,0.0340602962
IS4	C,0,3.1564694223,-0.6461337843,0.3050469065 C,0,4.2253081174,-1.3740818151,-0.037679419 C,0,5.4934007143,-0.6176530574,-0.2462363102 C,0,5.2721777488,0.6049756822,-0.6928722073 C,0,4.1880481898,1.3549554865,-0.7061579082 C,0,3.1392245596,0.9125367482,0.2970424202 H,0,2.2478495909,-1.124718012,0.6526507899 H,0,4.2141920745,-2.4563364726,-0.0054957389 H,0,6.4124945662,-0.9733598904,0.202787307 H,0,3.3635265717,1.2324199802,1.3220065574 H,0,3.8938783194,2.0281943998,-1.5027478524 N,0,1.8514795673,1.510829219,-0.0556676566 H,0,1.1370061426,1.2618107868,0.6177084027 H,0,1.5380676054,1.178819489,-0.9615562711
IS5	C,0,-0.1489471843,0.0861061409,-1.774217156 C,0,0.3774451373,-0.6746652966,-0.6255884157 C,0,0.3766078763,-0.0939578171,0.5804542971 C,0,-0.296678681,1.2562173999,0.7875320363 C,0,-1.3299408002,1.4408111587,-0.2828976684 C,0,-1.0033012764,1.103489171,-1.5712623615 H,0,0.2810997472,-0.1326954937,-2.7480808572 H,0,0.8886133172,-1.6174917044,-0.7808768002 H,0,0.9054515765,-0.5218718477,1.4217244216 H,0,-0.748898995,1.3256512982,1.779855595 H,0,0.4739228803,2.0366261069,0.7525643933 N,0,-2.576311565,1.802996451,0.0785794914 H,0,-2.836682304,1.9357167388,1.0395728753 H,0,-3.2931511289,1.8466792242,-0.6284455811
IS6	C,0,-1.2187251131,-1.2125620718,0.231979958 C,0,-1.8452878296,-0.0459421609,-0.2319032674 C,0,-1.1618660991,1.2002756121,-0.2132510908 C,0,0.1412946816,1.2760862461,0.1419207787 C,0,0.9288165305,0.0245845235,0.4176841363 C,0,0.1479879475,-1.2149743949,0.2957089925 H,0,-1.7939367863,-2.1235052609,0.3543422437 H,0,-2.8540173128,-0.0899942888,-0.6257151857 H,0,-1.7173021195,2.1007264008,-0.4439801103 H,0,0.6195248808,2.2328171579,0.3179689996 H,0,1.1368122402,0.0623985134,1.5165528161 N,0,2.1764381272,-0.031821672,-0.3592795679 H,0,2.8694177997,0.6156704203,-0.0011162189 H,0,2.5557940729,-0.9706820349,-0.2975174741
IS7	C,0,1.1617222361,0.7085100908,-0.5952658503

	C,0,1.5761412938,0.0058743914,0.682042551 C,0,2.365367781,0.7259184328,1.463266768 C,0,2.6680377,2.0287609316,1.3687088763 C,0,1.6754478655,2.8343366988,0.6768931396 C,0,1.0204841238,2.2167033064,-0.3446621375 H,0,0.1994613121,0.2978532149,-0.9126571211 H,0,1.0356108915,-0.8779617943,0.9983737006 H,0,1.8336760758,0.586378416,-1.4543067014 H,0,3.6373548445,2.4457806756,1.6180226612 H,0,1.5966853395,3.9060714795,0.817325845 N,0,0.3146053772,2.890645777,-1.3094719856 H,0,-0.422250861,2.409460459,-1.7954883332 H,0,0.1664377802,3.8791627203,-1.1918400625
IS8	C,0,0.5306647868,0.775957692,-0.2071616018 C,0,1.5662399763,-0.1317070754,-0.8038651391 C,0,2.8664032415,0.3565786842,-0.6677779197 C,0,3.1699166769,1.5599362647,-0.0276915004 C,0,2.2092563079,2.4642375758,0.4420130509 C,0,0.8754702762,2.1472578964,0.2887763247 H,0,-0.3818072425,0.7927437034,-0.812170146 H,0,0.2316781179,0.1979726792,0.6850091316 H,0,3.6990753876,-0.2252068555,-1.0520202357 H,0,4.2128864082,1.8361286947,0.1059384356 H,0,2.5109283776,3.4143342023,0.8652061612 N,0,-0.1206812531,3.0078220768,0.5744354073 H,0,-1.0821687447,2.74058109,0.4581613751 H,0,0.0647952833,3.9313794215,0.9280572661
IS9	C,0,1.0009322169,1.0796793567,1.2479694411 C,0,1.655396881,0.0306686757,0.7726803395 C,0,2.4713072941,-0.091171826,-0.2577757431 C,0,2.9512877959,1.2494333955,-0.7895115636 C,0,1.8620313728,2.3014372556,-0.6105765265 C,0,0.8398353824,2.1742034881,0.2644343515 H,0,3.1330391366,1.1010784078,-1.857966369 H,0,0.8538342187,1.3004957746,2.2994282643 H,0,2.5867142731,-0.9860013747,-0.8557248513 H,0,3.9051906039,1.6152155398,-0.3852251586 H,0,1.9622678349,3.2088536967,-1.1958071604 N,0,-0.1642286234,3.1188479701,0.4818408351 H,0,-1.0346786618,2.7354176597,0.8158978952 H,0,-0.3102819452,3.7789026702,-0.266782534
IS10	C,0,0.6929987852,0.9904231907,0.8936044355 C,0,1.4856775653,-0.1285113014,0.6843934467 C,0,2.6033070825,0.0823453443,-0.2841761541 C,0,2.8001965489,1.4056294412,-0.9393476184 C,0,1.9768033774,2.4272295731,-0.6687839441 C,0,0.8924244518,2.2310365669,0.2680571655

	H,0,2.5250362046,-0.693313933,-1.0615844902 H,0,-0.1501127715,0.9366899835,1.5845120517 H,0,3.5397337357,-0.212677194,0.2140335438 H,0,3.6183665008,1.5384933615,-1.640666686 H,0,2.0981338432,3.4000303622,-1.1317616902 N,0,0.0866798521,3.2794667405,0.5146902798 H,0,-0.6802523707,3.1893924637,1.1591698056 H,0,0.2236549747,4.1708261608,0.0707410743
IS11	C,0,0.1042694511,1.1896018226,0.0382377191 C,0,0.7687287609,-0.0304767312,-0.0165894737 C,0,0.2557192218,-1.3010700701,-0.0507932342 C,0,-1.154217055,-1.302032115,-0.024033775 C,0,-1.9056709999,-0.1299908795,0.0305722032 C,0,-1.2828615416,1.1204437663,0.062025913 H,0,0.6113864896,2.1486035259,0.0619126719 H,0,2.446040566,-1.0687077124,-0.0836304559 H,0,-2.9888802302,-0.178913006,0.0494033386 H,0,-1.8704427569,2.0277972906,0.1045996009 N,0,2.292221006,-0.0452044836,-0.0459216757 H,0,2.6953031624,0.4025150766,-0.8703063448 H,0,2.726991828,0.3464484316,0.7908062699 H,0,-1.6906159122,-2.2465499158,-0.0462797473
IS12	C,0,-0.4840328763,0.9444882796,-0.3641919234 C,0,0.3075985914,-0.1870216267,-0.4194728673 C,0,0.6759400477,-0.9456611803,0.678674348 C,0,0.2578532266,-0.6100182077,1.9772012921 C,0,-0.5505519727,0.5486308191,2.0178338591 C,0,-0.9202024446,1.3113148877,0.9086130922 H,0,-0.7504391259,1.511710808,-1.248176144 H,0,1.3094692972,-1.8242744465,0.5032350717 H,0,-0.9241097781,0.8889814188,2.9818173291 H,0,-1.545666963,2.1915641586,1.0187294088 N,0,0.8108307112,-0.6329244135,-1.7771106034 H,0,1.398669039,0.073334101,-2.2250234129 H,0,1.3740413635,-1.4735006912,-1.6343082889 H,0,0.048572524,-0.8641573669,-2.417817251
IS13	C,0,3.0132320706,-1.5479528954,0.1908357607 C,0,3.6302984255,-0.9667287493,1.3733950072 C,0,3.1579518017,0.1686787348,1.8973168267 C,0,2.0066216804,0.9040460817,1.2845282193 C,0,1.2540394686,0.1585551997,0.1956224633 C,0,1.9122961474,-1.018824219,-0.3719221642 H,0,3.4538760549,-2.4436565317,-0.2297091817 H,0,4.4795735979,-1.470402794,1.8155872138 H,0,3.6227020692,0.6087033372,2.7710460595 H,0,2.3891645929,1.8338177718,0.842204689 H,0,1.4490794282,-1.4841317439,-1.2340749754

	N,0,0.1075890348,0.599180716,-0.1592780875 H,0,1.2953181921,1.2324664344,2.0449433531 H,0,-0.2797212041,0.0409075178,-0.9208063137
IS14	C,0,1.3622956196,-0.2269123944,-0.5357204461 C,0,1.120717435,-1.2884588206,0.2853511727 C,0,-0.1512791282,-0.7732540732,0.8261288806 C,0,-1.4054135332,-1.0360869247,0.095432292 C,0,-1.309154192,0.0399775104,-0.7365646479 C,0,0.0432938075,0.4125627362,-0.1861447894 H,0,2.1441270623,0.0462025925,-1.2306837691 H,0,1.6182149695,-2.2440484623,0.402506357 H,0,-2.0929366989,-1.8732876451,0.1234955774 H,0,0.9203383383,1.7634194399,1.1211116277 N,0,0.1299695885,1.777658553,0.4749661244 H,0,0.2561961577,2.540819359,-0.1898677536 H,0,-0.734530035,1.9287482664,0.9966957708 H,0,-1.9102973865,0.4512579113,-1.5355023881
IS16	C,0,0.0657750725,-0.5342578378,-0.8746488163 C,0,1.1447440485,-0.4551313443,-0.027708123 C,0,1.2155806464,0.4844420343,1.0319533413 C,0,-0.0723137702,1.1645773697,1.3001636836 C,0,-1.2835939784,0.8988281778,0.4843322219 C,0,-1.188906284,0.117271098,-0.620003611 H,0,0.1339757571,-1.1332656378,-1.7805806753 H,0,2.0109906538,-1.0703854482,-0.2518842715 H,0,-0.28389153,1.006270226,2.3720437292 H,0,0.1480697976,2.2449539984,1.3076255852 H,0,-2.2328649809,1.3368910324,0.7758713529 N,0,-2.2226904941,-0.0758289958,-1.5418618369 H,0,-2.2501757719,-0.9847837279,-1.9782324275 H,0,-3.1364207763,0.2105802954,-1.2248610225
IS18	C,0,0.0067824973,-1.0857458524,0.2662556053 C,0,1.4569098604,-0.8436533529,0.0210067964 C,0,1.9013239502,0.3538960861,-0.392321 C,0,1.0520940549,1.5341246347,-0.5369264819 C,0,-0.3257979007,1.2833240763,-0.4544437902 C,0,-0.8748117998,0.0753017173,-0.0612750387 H,0,-0.3189830585,-1.9643545904,-0.3036327226 H,0,2.1262320205,-1.6778865111,0.2056188604 H,0,2.9650450771,0.4711645751,-0.5772869739 H,0,-0.1498615574,-1.3584064648,1.3187225258 H,0,-1.0271226972,2.1026933985,-0.6187924666 N,0,-2.2023123614,-0.101579903,0.1013104583 H,0,-2.8352389024,0.6640050359,-0.0578497008 H,0,-2.5867921929,-0.9480628592,0.4827629184
IS19	C,0,-0.3721855223,0.0613576757,-1.7567157593 C,0,0.6541272122,-0.1961191585,-0.9085181556



	C,0,0.6316507756,0.3326841233,0.4683065744 C,0,-0.6410460235,0.9732029556,0.8697060684 C,0,-1.693356759,1.0839390816,0.0028657899 C,0,-1.4755769083,0.8956824032,-1.4041302925 H,0,-0.2994991464,-0.2846201883,-2.7835122671 H,0,1.5416047837,-0.7276260511,-1.2345924863 H,0,0.896150234,-0.4733546501,1.170920629 H,0,-0.6826720631,1.4128633936,1.8618253746 H,0,1.4627287229,1.0457961691,0.5860889771 N,0,-2.9534317424,1.5031015695,0.3896672826 H,0,-3.0593497028,1.9327939893,1.2949869876 H,0,-3.4898758604,1.9256939171,-0.3525139927
IS20	C,0,-0.220023231,0.4973178546,-1.7569576598 C,0,0.8334008883,0.1927917259,-0.7233223331 C,0,0.2456891094,-0.0521206443,0.634509961 C,0,-1.0247264331,0.2565604028,0.9276161666 C,0,-1.7410175698,1.0533977375,-0.0681714992 C,0,-1.442177953,0.9366953387,-1.4162173464 H,0,0.0269845895,0.2272373719,-2.7809986629 H,0,1.3716905418,-0.7079120796,-1.0428980415 H,0,0.8915238153,-0.4772637705,1.3938637235 H,0,-1.4435936869,0.0665819077,1.9105034941 H,0,1.6225624383,0.954823322,-0.6342357536 N,0,-2.6330692467,1.9627030142,0.3755526275 H,0,-2.7479643608,2.1636821009,1.3537370077 H,0,-3.0564272514,2.5776272582,-0.301783224
T1/2	C,0,0.6880721209,0.0961393344,-1.2874426468 C,0,1.6665291454,-0.1210387089,-0.3793697071 C,0,1.4412890571,0.3545172187,0.9817820872 C,0,0.8451762484,1.6691629529,1.0560951341 C,0,-0.1615871998,1.9141845059,0.1790688346 C,0,-0.4403964381,0.7076682274,-0.5829503072 H,0,0.6238354323,-0.376870056,-2.2558815973 H,0,2.5337113225,-0.7258387215,-0.6090979961 H,0,2.1417396723,0.0565925224,1.750139837 H,0,1.0441258533,2.3247739562,1.8934665902 H,0,-0.9128551814,2.674982808,0.3282056582 N,0,-1.214896414,-0.1137520407,0.1336348302 H,0,-1.2703331354,-1.037774653,-0.2986202055 H,0,-0.1259391434,-0.2616286358,0.9734212586
T1/3	C,0,-0.3327285873,-0.6878458626,-0.3262391076 C,0,1.1107123027,-0.8793758576,-0.2267691179 C,0,1.8788456083,0.2176609627,0.0031706623 C,0,1.2843960564,1.4901401706,0.1821253698 C,0,-0.0905648647,1.6617443434,0.1778390612 C,0,-1.0078705879,0.5678270175,-0.0123850808 H,0,-0.944555147,-1.5864088971,-0.280580392

	H,0,1.5436730767,-1.8617255505,-0.3597030989 H,0,2.9569570797,0.136279339,0.0554722871 H,0,1.9370613677,2.3437008963,0.3389584205 N,0,-0.6660918337,2.9012458318,0.3836064839 H,0,-0.5614296145,-0.2718595443,-1.3738600056 H,0,-0.1595516811,3.6004286572,0.9013960821 H,0,-1.6607233353,2.8728252236,0.5443607159
T1/4	C,0,-1.0806735903,-0.8984008684,0.3856740276 C,0,-2.0856014215,-0.033383983,0.9988798209 C,0,-3.3985999497,-0.6815553263,0.7600561891 C,0,-3.3521528406,-0.4585637651,-0.5745416863 C,0,-2.574371232,-1.1517335353,-1.5060375064 C,0,-1.3328059693,-1.4202790258,-0.8805860004 H,0,-0.1138869954,-1.0155278372,0.8586040633 H,0,-0.5379805697,-1.9023865345,-1.4358844689 N,0,-1.7796913278,0.7365619827,2.1354243856 H,0,-0.9675564436,1.3290281702,2.0343408113 H,0,-2.5662057804,1.2552846607,2.4953961073 H,0,-2.7241268777,-1.2221231981,-2.5732655656 H,0,-3.8067530667,-1.5614006825,1.2490696357 H,0,-2.4622335754,0.5725912926,-0.2156775932
T1/6	C,0,-1.22800726,-1.2236383301,-0.1565713468 C,0,-1.8740472771,-0.0232710205,-0.3373773527 C,0,-1.1867704795,1.2205407646,-0.2823757242 C,0,0.1426216081,1.228621697,-0.0157998025 C,0,0.8183525207,-0.0360704279,0.3235780381 C,0,0.1680826683,-1.3448658839,0.1163233276 H,0,-1.8022726343,-2.1350581748,-0.2907592028 H,0,-2.9363506087,-0.0117089307,-0.5604972494 H,0,-1.7201659916,2.138634057,-0.4895482791 H,0,0.7249450348,2.1410644008,-0.0087871249 H,0,0.4708755414,-0.1986922226,1.3932965097 N,0,2.2783123778,0.0541032989,0.2931441802 H,0,2.6731916848,-0.3079716956,1.1528114392 H,0,2.6117428653,-0.5714672423,-0.4322350223
T1P8	C,0,0.1109222656,1.5314181938,-0.172715804 C,0,1.3700700748,1.0820221835,0.0202858069 C,0,0.9710361199,-0.3465084829,0.2101311752 C,0,0.7921232649,-1.2524151368,-0.9650562411 C,0,-0.4894474016,-0.8937305365,-1.1970513708 C,0,-0.4866243435,0.1462315561,-0.1022066771 H,0,-0.3355254447,2.5038719084,-0.3341078234 H,0,2.3340997141,1.5760250301,-0.0072501077 H,0,1.4689445892,-1.9207893147,-1.4840846283 H,0,-0.0645078362,-0.6033473033,1.4281978388 N,0,-1.1955333138,-0.2274717255,1.1987076577 H,0,-1.534500375,0.5548260983,1.743451469

	H,0,-1.9024638175,-0.9459597133,1.1110304611 H,0,-1.2538735062,-1.2040377571,-1.8973247763
T1/7	C,0,-1.7399127423,-0.3515954505,-1.2405465498 C,0,-1.1774952472,0.4001355865,-0.1342166367 C,0,-2.0653083217,0.9364239973,0.8246364988 C,0,-3.4488012366,0.7599871946,0.6417845552 C,0,-3.6513710403,-0.1273845921,-0.4241727765 C,0,-2.8277326325,-1.1789260148,-0.6632239387 H,0,-1.0893514948,-0.6323970963,-2.0713383366 H,0,-2.9151636243,0.4791180257,-1.4246639286 H,0,-2.7230567933,-2.065033885,-0.0441329052 N,0,0.1822095409,0.6612022426,-0.0882219759 H,0,0.7034966343,0.4602259581,-0.9265548629 H,0,0.4749412773,1.5077547882,0.3728356833 H,0,-4.1688427924,1.4514603571,1.0604737863 H,0,-1.6963839672,1.6631833686,1.5391419774
T1/8	C,0,-0.9591609798,0.0424596701,0.0988524975 C,0,-0.0947341698,1.2025596889,-0.0314649882 C,0,1.3473425657,1.1495127511,-0.1149000965 C,0,1.8447685743,-0.1825110059,-0.2072698517 C,0,1.0385123373,-1.2918334323,-0.0701941382 C,0,-0.3579482081,-1.1965087567,0.0721878031 H,0,0.4208340195,1.410420814,-1.1233471244 H,0,2.9111623957,-0.3297703537,-0.3356449074 H,0,-0.5581216966,2.1727895954,0.1452736536 H,0,1.4783321369,-2.2839436927,-0.0783508642 H,0,-0.9550897119,-2.0955673103,0.1665029384 N,0,-2.3146409635,0.2208003574,0.2016402382 H,0,-2.6583189549,1.123048885,0.483769918 H,0,-2.8872323248,-0.5583322203,0.4803199318
T1/9	C,0,-1.4482853286,1.0755243549,-0.2618518435 C,0,-1.78931892,-0.0603840858,0.6371341889 C,0,-1.2035326651,-0.9702767844,-0.1720927605 C,0,0.1905931673,-1.1411744192,-0.160968097 C,0,0.7922594031,0.1296156746,0.0386529807 C,0,-0.0496510895,1.2706307408,-0.0350264273 H,0,-1.7855883792,-0.0677162212,1.7227742828 H,0,-2.1059573661,1.8924763705,-0.5457042325 H,0,-1.4262030706,-0.072490139,-1.1889174234 H,0,0.7433508264,-1.9329790782,-0.649906309 H,0,0.3957630879,2.255171528,-0.1168497562 N,0,2.1748524051,0.2668464515,-0.0055966439 H,0,2.7048820654,-0.4633733281,0.4400176146 H,0,2.5427208738,1.1845279358,0.1817164363
T1/10	C,0,-0.0716809654,-0.3228694544,-0.575848891 C,0,1.0167771196,-1.2655357302,-0.7023006688 C,0,1.9884350213,-1.4827066552,0.3417548874

	C,0,1.8542830436,-0.5984927729,1.4391748322 C,0,0.7796321015,0.2636735095,1.6105955672 C,0,-0.18078436,0.4098552874,0.5577675262 H,0,-0.791837783,-0.2050480221,-1.3768962238 H,0,0.963410476,-1.9852178071,-1.51477323 H,0,2.1498685634,-0.8355489858,-0.8975089481 H,0,2.5959069272,-0.6379347327,2.2341782323 H,0,-0.9883567987,1.1226159032,0.6808728058 N,0,0.6333166233,1.0354564581,2.7335530826 H,0,-0.2590628531,1.4536137718,2.9326697342 H,0,1.1997441244,0.8217048704,3.5365778538
T1/11	C,0,-1.3396812402,-0.3097278859,-1.6108660394 C,0,-1.2912940138,0.8089866607,-0.797375687 C,0,-2.257789055,1.2611571976,0.088221159 C,0,-3.411082525,0.468147382,0.1434335374 C,0,-3.52830013,-0.6751922495,-0.6496970563 C,0,-2.5073309216,-1.0646859995,-1.5189462378 H,0,-0.5390909948,-0.5990461507,-2.2803840208 H,0,-0.9608878027,2.2769856601,0.119386234 H,0,-4.4271337023,-1.2786774548,-0.5957243581 H,0,-2.6209393714,-1.9546683065,-2.1236949278 N,0,-0.1937002919,1.8027631833,-0.6702432041 H,0,0.6808776471,1.447863732,-0.2872806193 H,0,-0.0047126912,2.3603941884,-1.5014061744 H,0,-4.2315203372,0.729688753,0.8032809248
T1/13	C,0,0.2741573302,1.8378119745,0.8436606571 C,0,1.6605624852,2.1689008562,0.9738603765 C,0,2.1843047521,3.1658434489,0.1965921917 C,0,1.3409889782,3.9335311744,-0.662033145 C,0,0.0158051297,3.6436794366,-0.8666654388 C,0,-0.4463432638,2.4381807261,-0.2758059947 H,0,-0.2920183876,1.8043987519,1.7755829204 H,0,2.2672440646,1.6890298034,1.732028438 H,0,3.2270216436,3.438992148,0.2816311576 H,0,1.7795841501,4.7696533332,-1.1935327958 H,0,-0.5894813067,4.2102582512,-1.5618763724 N,0,-1.3337580782,1.5346461255,-0.650366358 H,0,-0.6151680869,0.8337612299,0.3381878643 H,0,-2.1657847305,1.8097096202,-1.173124041
T1/16	C,0,-0.2177784623,0.9202430459,0.3114068838 C,0,1.1262096588,1.4893692648,0.3631458001 C,0,1.4833827979,2.8102109107,-0.1542994693 C,0,0.305897433,3.5563347399,-0.509538216 C,0,-0.966468311,3.0570487016,-0.4674880648 C,0,-1.2604125197,1.7127002225,-0.0701713313 H,0,-0.3795209052,-0.1129733387,0.5977095058 H,0,1.9350860736,0.7678964689,0.4586704178

	H,0,1.2424243338,2.1244842957,1.3182927458 H,0,0.4362444774,4.5689705094,-0.878238113 H,0,-1.8041558759,3.6870480161,-0.7569186993 N,0,-2.5896102,1.3006513221,-0.0530083492 H,0,-2.7420961484,0.3048625284,-0.0219548201 H,0,-3.2038240119,1.7628562627,-0.7047600002
T1/18	C,0,-0.7781343172,1.7634762178,0.7975879454 C,0,-0.0127279126,0.4950769347,0.5294309463 C,0,1.1729040188,0.9139409188,0.0683092391 C,0,1.1223739951,2.3798533962,0.1842640812 C,0,0.2423326969,2.9908521517,-0.8501965655 C,0,-0.9821189349,2.636782611,-0.4327335324 H,0,-1.5814325655,1.7643285447,1.5331857933 H,0,-0.3744455844,-0.5065878881,0.7008969325 H,0,1.9980020006,0.3696431996,-0.3658884752 H,0,0.1355035715,2.4121045614,1.3149351548 H,0,0.5676644365,3.6248880303,-1.6586808695 N,0,-2.2539691851,3.0881503153,-0.7785312177 H,0,-2.3113895102,3.5381754709,-1.6804784806 H,0,-2.9815073096,2.3951558657,-0.6724535817
T1/19	C,0,0.2211445269,0.3356598101,0.1752488051 C,0,0.5504523989,-0.885262294,-0.2643216575 C,0,-0.2900078831,-1.1072507661,-1.5154699907 C,0,-1.7829749456,-1.0746380533,-1.2695568446 C,0,-2.0101516103,0.1596532901,-0.7943113144 C,0,-0.6967817444,0.8574698878,-0.848998512 H,0,0.5539661473,0.8854457985,1.0419050639 H,0,1.2989874608,-1.5639346797,0.1159962582 H,0,0.082230855,-1.8074597083,-2.2612889356 H,0,-2.4549679861,-1.9112660988,-1.37647217 H,0,-0.1540598832,-0.0260799162,-2.0217286221 N,0,-3.0696531554,0.7765659165,-0.1588839158 H,0,-3.930104137,0.2515494524,-0.1351904575 H,0,-3.2160219839,1.744268751,-0.402972387
T1/20	C,0,-1.0213917038,-0.7194583002,-1.0882632053 C,0,0.1889300397,-0.5748409741,-0.2561462403 C,0,0.5400631569,0.8335006695,-0.3425584287 C,0,-0.4523232507,1.8032239144,-0.3670362431 C,0,-1.8126746364,1.3950121268,-0.2168307237 C,0,-1.863240974,-0.0066206393,-0.2950161731 H,0,-1.0720916654,-0.8122252656,-2.1706370311 H,0,0.9768689726,-1.3167412356,-0.1452650373 H,0,1.5808043424,1.1275166388,-0.2807082967 H,0,-0.1923737034,2.8528132608,-0.2966262058 H,0,-0.886556887,-0.3539447265,0.673011932 N,0,-2.8085265404,2.2549875719,0.198426967 H,0,-3.7036879498,1.8357382958,0.3848605183

	H,0,-2.5602928106,2.9855637034,0.8471700877
T1P1	C,0,0.9979141711,-0.8422433327,-0.6633968654 C,0,2.1813390698,-0.440650032,-0.1650815136 C,0,2.0033830534,0.6477416302,0.8130074956 C,0,0.9754713377,1.4681597819,0.5335354459 C,0,-0.0014562279,1.401371435,-0.4374192304 C,0,-0.2225270009,0.0023177982,-0.3540042173 H,0,0.8875509214,-1.7240369704,-1.28396365 H,0,3.1119916304,-0.9672449387,-0.3315544808 H,0,2.3844012686,0.5286000437,1.8182730401 H,0,0.0316282416,1.0230836857,1.7940432753 H,0,-0.7571834873,2.1515650201,-0.6111370715 N,0,-1.1763110315,-0.3576848916,0.5008637898 H,0,-1.1679132898,-1.3538285176,0.7249872768 H,0,-0.6904048666,0.3083098482,1.5647169554
T1P2	C,0,0.1863784489,1.3058537298,-0.2390840624 C,0,0.6322493903,-0.0280092871,-0.4747834779 C,0,1.3735794293,-0.8948879896,0.4975477587 C,0,0.0290670558,-0.811525404,0.7543545377 C,0,-0.8186075792,0.0925837819,1.4961878406 C,0,-0.6702017208,1.329095841,0.8968338578 H,0,0.2654541066,2.113775339,-0.9536381222 H,0,2.2134838072,-0.665871516,1.1393569252 H,0,-1.3596840984,-0.1269305551,2.4011802072 H,0,-1.1323996038,2.2345462173,1.268445999 N,0,0.171346606,-0.800795746,-1.7045182182 H,0,-0.4105572988,-0.2629804736,-2.33692398 H,0,0.9132511972,-1.3003781879,-2.1803032744 H,0,-0.3853877903,-1.2520103996,-0.5646530111
T1P5	C,0,-1.3396812402,-0.3097278859,-1.6108660394 C,0,-1.2912940138,0.8089866607,-0.797375687 C,0,-2.257789055,1.2611571976,0.088221159 C,0,-3.411082525,0.468147382,0.1434335374 C,0,-3.52830013,-0.6751922495,-0.6496970563 C,0,-2.5073309216,-1.0646859995,-1.5189462378 H,0,-0.5390909948,-0.5990461507,-2.2803840208 H,0,-0.9608878027,2.2769856601,0.119386234 H,0,-4.4271337023,-1.2786774548,-0.5957243581 H,0,-2.6209393714,-1.9546683065,-2.1236949278 N,0,-0.1937002919,1.8027631833,-0.6702432041 H,0,0.6808776471,1.447863732,-0.2872806193 H,0,-0.0047126912,2.3603941884,-1.5014061744 H,0,-4.2315203372,0.729688753,0.8032809248
T2P6	C,0,4.032856554,-0.4363991998,0.5654775317 C,0,4.3703871022,0.6291228435,-0.3692174237 C,0,3.3995924664,1.2859049598,-1.0638208063 C,0,2.1082923409,0.7209281346,-1.04088675

	C,0,1.6702032995,0.0203345639,0.1032008886 C,0,2.6132854349,-0.6595275469,0.8124805226 H,0,2.334439129,-1.4223466448,1.5308884027 H,0,5.4231861325,0.8134582776,-0.5402294695 H,0,3.6493630156,2.0726533596,-1.765049115 H,0,0.6334980954,2.6452343724,-1.0751869808 H,0,0.613189647,-0.1239174384,0.2915498057 N,0,4.9969239368,-1.0886646302,1.1311419476 H,0,0.8869656768,2.0058600441,-1.4238650726 H,0,4.6307978891,-1.7942832855,1.771808259
T3P4	C,0,-1.0299360634,-0.9809838706,-0.1849177031 C,0,-1.8189429321,0.1385262406,0.0700764419 C,0,-1.0346146365,1.265323659,0.2638830172 C,0,0.3610882542,1.1812525588,0.1934766796 C,0,1.0135900806,-0.0325776495,-0.0760323854 C,0,0.2605582347,-1.2160603767,-0.2862574797 H,0,-1.8691430923,-1.9751007074,-0.7772634527 H,0,-2.8982773354,0.139875937,0.113549649 H,0,-1.503695171,2.2175047533,0.4730162862 H,0,0.9436428984,2.0819270204,0.3569666737 N,0,2.3981841924,-0.0993828952,-0.0966356437 H,0,-1.8342227398,-2.1396382802,0.0350555712 H,0,2.9135067866,0.74467902,-0.2855948395 H,0,2.7734975234,-0.9294363993,-0.5249868146
T4P2	C,0,-1.2894128315,-0.4388292883,-1.0142328646 C,0,-1.2900845744,0.6853439875,-0.1684776412 C,0,-2.478825092,1.1463491385,0.4670611141 C,0,-3.5554028301,0.4566238815,0.0412585194 C,0,-3.6718898618,-0.5337028135,-0.8709692716 C,0,-2.4537732724,-1.1210761685,-1.2989210229 H,0,-0.348393257,-0.7689058743,-1.4321609758 H,0,-0.3260549463,1.0942820548,0.1897468312 H,0,-2.4364788771,1.7968525816,1.3291839997 H,0,-4.6078062659,-0.7872991027,-1.3542725911 H,0,-2.451169285,-1.9957997148,-1.9378884024 N,0,0.3425158711,2.0875285378,-1.0740649132 H,0,0.1396910684,1.703928462,-1.9992130135 H,0,-0.2815158961,2.8959725885,-1.0115656082
T5P12	C,0,-0.8391711239,-0.7081590679,-1.40209471 C,0,0.4977373103,-0.6505576262,-0.9554135716 C,0,0.7608562224,0.2426783702,0.0630383598 C,0,-0.2602920676,1.1132129254,0.4441327805 C,0,-1.553020451,1.2062206351,-0.0564023047 C,0,-1.7615819117,0.2211106362,-0.9981327272 H,0,-1.146910836,-1.5403716868,-2.0281272969 H,0,1.2635907543,-1.3253028567,-1.3189355446 H,0,1.7251978807,0.2954891024,0.5472838112

	<p>H,0,0.0824098798,1.4322534841,2.0214724608  H,0,0.1074069874,1.976406272,1.3001403729  N,0,-2.463903797,2.1955598014,0.2656753143  H,0,-2.0957730064,3.0999898458,0.5164259693  H,0,-3.2473172712,2.2350816549,-0.3701486338</p>
T6/5	<p>C,0,-1.1364649924,-1.2371816387,0.016479369  C,0,-1.8455958766,-0.0326028119,-0.1062022003  C,0,-1.1891594424,1.18412659,-0.0399842962  C,0,0.2023312532,1.191925157,0.0732434642  C,0,0.9299624803,-0.0715230553,0.032294639  C,0,0.2581822587,-1.3490587418,0.060336625  H,0,-1.7256499661,-2.1501427644,0.0438817428  H,0,-2.9259035007,-0.0453929469,-0.1984402631  H,0,-1.7297666202,2.1196681362,-0.0274291655  H,0,0.7518779052,2.1206915301,0.1835629442  H,0,0.517475567,0.2936582777,1.1723130496  N,0,2.2992820108,-0.0600674057,-0.1779031051  H,0,2.8246500497,0.7821762627,-0.0078935746  H,0,2.7537298733,-0.923199589,0.079135771</p>
T7P7	<p>C,0,0.2580667481,1.1469043004,0.255805304  C,0,-1.1065070229,1.2967210297,-0.1931412287  C,0,-1.8594632781,0.1670952417,-0.090795728  C,0,-1.4062158148,-1.0951941624,0.1197105691  C,0,0.0088825644,-1.3161939248,-0.0918485249  C,0,0.7537661085,-0.2126775952,0.1538977944  H,0,0.7373826702,1.7849517332,1.0094660368  H,0,-1.4551269224,2.2071063366,-0.667852681  H,0,1.623922616,1.131832783,-0.3741378843  H,0,-2.0245395132,-1.8784271473,0.5459909361  H,0,0.4517190628,-2.2622540304,-0.3858626219  N,0,2.206902797,-0.0243772567,-0.1080972666  H,0,2.8352496045,-0.2452449489,0.6601574867  H,0,2.5228313797,-0.4773123586,-0.9575371917</p>
T7P11	<p>C,0,-0.1651620423,0.1850101183,-1.598210973  C,0,1.0059301464,0.8712994826,-1.5864446794  C,0,1.4407080928,1.7651919283,-0.644307259  C,0,0.5342989309,2.2562489719,0.3011028068  C,0,-0.6880158863,1.5908882618,0.421109655  C,0,-0.9902161274,0.6122653792,-0.54619548  H,0,-0.5394035186,-0.4327861188,-2.4039803425  H,0,-2.1281935277,-0.4969907338,0.3329797666  H,0,2.4849671015,2.0513178086,-0.5816009494  H,0,0.8001457536,3.0442322855,0.9990495305  H,0,-2.0745431038,0.1613376292,-0.5007826956  N,0,-1.6061420971,1.9385589828,1.4008674955  H,0,-1.2273080856,2.4384512538,2.1894619478  H,0,-2.2415626464,1.2043399907,1.6778086867</p>



T8P4	C,0,-1.2415249012,-0.4811139912,-0.8299620962 C,0,-0.0605405771,-1.2229585175,-0.6259615193 C,0,0.9986957131,-0.6526555106,0.0756545743 C,0,0.9375605644,0.6448176736,0.6029586327 C,0,-0.2087527728,1.4208555943,0.4302046364 C,0,-1.1778298214,0.7234040747,-0.3019409216 H,0,-2.4422058442,1.4023701628,-0.1211137342 H,0,0.0419978643,-2.23306782,-1.0068803509 H,0,1.9084973216,-1.2221501494,0.2341313744 H,0,1.7783015818,1.0539160349,1.1493073233 H,0,-2.0885456616,1.6809424749,-0.8256512851 N,0,-0.325277651,2.7331265196,0.8661898161 H,0,-1.2508859165,3.0435306393,1.1194487851 H,0,0.3620403705,3.0206659346,1.5447724349
T9P3	C,0,0.8847823624,-1.8761112043,-0.2688440153 C,0,2.1076498026,-2.4415326143,0.1028783102 C,0,2.9572564129,-1.4452477038,0.4962603337 C,0,2.7250867195,-0.0998055096,0.5142810877 C,0,1.4045486503,0.3832016316,0.3371907106 C,0,0.5041118258,-0.5368800818,-0.1936185562 H,0,2.2573284814,-3.5047067672,0.2332676774 H,0,0.0242558722,-2.6403202725,-0.6210946316 H,0,0.0377281014,-2.4620551972,-1.5855732435 H,0,3.5434064999,0.6124230637,0.5729949066 H,0,-0.483204299,-0.2383589932,-0.5177644409 N,0,1.0785048304,1.7190839125,0.5284353955 H,0,1.6534282066,2.2228579932,1.1832416637 H,0,0.1004810636,1.9399672529,0.6210412321
T10P10	C,0,-1.0360363434,-0.3673891975,0.5337271747 C,0,-0.0257365313,-0.7979904144,-0.3098148122 C,0,0.9220004469,-0.1811628685,-0.9757230152 C,0,0.9005055556,1.2025052406,-0.7774734971 C,0,-0.0629669326,1.8021519595,0.0568645333 C,0,-1.0325875929,1.0032278234,0.711813751 H,0,-0.3736922467,-2.1639910425,-0.7484860862 H,0,0.1339033409,-2.2442311422,-0.1053821697 H,0,-1.7669376661,1.4667854756,1.358054616 H,0,1.6246761311,1.8550141816,-1.2612439052 H,0,-1.7577388065,-1.0166317965,1.0132951832 N,0,-0.0449891401,3.1671041547,0.2850753253 H,0,0.476834185,3.726311354,-0.3695315379 H,0,-0.8980979402,3.6007140721,0.5959191001
T11P5	C,0,-0.1217083542,1.2125123522,-0.148668197 C,0,-0.6056612398,-0.0545450782,0.0193942189 C,0,-0.0829767782,-1.1999610369,0.1840073226 C,0,1.320679251,-1.2257265765,0.2054963413 C,0,1.9843790929,-0.0042636421,0.0462216577

	C,0,1.2813809869,1.1945782963,-0.1278382625 H,0,-0.695406984,2.118205956,-0.2810954476 H,0,-2.9614481386,-0.6834026296,-0.8153743095 H,0,3.0677740768,0.0212286087,0.0569351037 H,0,1.8214696902,2.1251101741,-0.2489619233 N,0,-2.8080852757,-0.0841462939,-0.013872507 H,0,-2.9464208485,-0.6326358285,0.8256753268 H,0,-3.4691640659,0.6855449541,-0.0326754066 H,0,1.8911755875,-2.1382032558,0.3383950825
T12P2	C,0,-0.4456515182,0.8873538536,-0.356584389 C,0,0.3274644552,-0.2388048654,-0.306771891 C,0,0.7426404384,-1.0451057552,0.6962222189 C,0,0.2298283018,-0.5541163145,1.9033342481 C,0,-0.5700025365,0.5815326799,1.9944136505 C,0,-0.9300340449,1.331580607,0.8782616161 H,0,-0.668965705,1.4004252767,-1.2806324751 H,0,1.3674015891,-1.9270348063,0.6000645356 H,0,-0.927924402,0.8967122841,2.9702640554 H,0,-1.5542197262,2.2196445842,0.9404997994 N,0,0.9229628698,-0.712709078,-2.1744061041 H,0,1.4808291712,0.0325133565,-2.5756431214 H,0,1.4890896168,-1.5479071027,-2.0869471144 H,0,0.1255633304,-0.90643838,-2.769541329
T13P1	C,0,0.9780904584,1.3762723,-0.1875515975 C,0,1.6858144785,0.1512884103,-0.0850673796 C,0,0.9835228718,-1.0370595626,0.0455575873 C,0,-0.3711576964,-1.0509156321,0.224255049 C,0,-1.1121810938,0.1982528678,0.2957838101 C,0,-0.3675237268,1.4152999124,0.0273329802 H,0,1.5282729267,2.294206097,-0.3501370804 H,0,2.7671249563,0.1588435358,-0.0630617441 H,0,1.4537438675,-2.0539289884,-0.1007156144 H,0,-0.9277242905,-1.977954906,0.2491725198 H,0,-0.907617393,2.3536583256,0.0215956773 N,0,-2.3972849107,0.1313044347,0.4924931032 H,0,1.1720214677,-3.2994852173,-0.7238511146 H,0,-2.8267229157,1.0537434428,0.3968868038
T13P9	C,0,2.2269763127,2.2434755902,0.7777610764 C,0,2.9261538435,2.6800860892,-0.3072628149 C,0,2.1296051748,3.189960434,-1.3352617742 C,0,0.7465344766,2.8856535124,-1.3870151201 C,0,0.1397128658,2.1658551438,-0.4068582155 C,0,0.8974179564,1.7008051936,0.7642532112 H,0,3.2682060824,1.3549823575,1.9410584968 H,0,3.9890064552,2.8853408444,-0.2697597757 H,0,2.5531061848,3.9051013883,-2.0295564563 H,0,3.694493529,0.7184752595,2.0260184048

	H,0,-0.8474947079,1.7412591158,-0.552429094 N,0,0.4703691497,0.8359271852,1.6295878544 H,0,0.1827380931,3.1865958599,-2.2609724653 H,0,-0.5008953661,0.5940737062,1.4360628123
T14P8	C,0,1.3817403013,-0.1774602146,-0.6042793331 C,0,1.1666734638,-1.1891553843,0.3540906091 C,0,-0.1394186527,-0.7427585247,0.7088951409 C,0,-1.4405952999,-0.928677446,0.1580716517 C,0,-1.3081212963,0.0912691213,-0.806507762 C,0,0.051745911,0.3308922778,-0.407094104 H,0,2.1571970437,0.0056062754,-1.333664458 H,0,1.7241500486,-2.0932310489,0.5765953237 H,0,-2.1917134245,-1.7020185823,0.2821939616 H,0,0.9212671013,1.9472917023,1.3283187595 N,0,0.1401260049,2.0415313218,0.6905194956 H,0,0.2656340499,2.8516938236,0.0977005722 H,0,-0.7299331626,2.1122540746,1.204178679 H,0,-1.915705476,0.4125076528,-1.6398722862
T16P10	C,0,1.2244584804,-2.1484322219,-0.0945667527 C,0,2.1185182643,-2.0210515886,0.8640603074 C,0,2.5638352199,-0.6750599667,0.9186296566 C,0,2.0831549904,0.2962214439,0.0524338835 C,0,1.1125261619,0.0113005311,-0.9364597715 C,0,0.6412609086,-1.2940679874,-1.0281102277 H,0,0.3969572349,-3.3029825403,-0.0053935662 H,0,1.0027420105,-3.4803398067,-0.5486173446 H,0,3.3051689912,-0.3746337665,1.6529958771 H,0,2.4578058949,1.3129661371,0.1225094046 H,0,-0.0977770828,-1.6022265316,-1.7573701274 N,0,0.6963561497,1.0049129148,-1.8279795103 H,0,-0.2000661044,0.8499853222,-2.2622347345 H,0,0.7821792305,1.9484477306,-1.4838928543
T18P2	C,0,0.1339058933,-1.1705077357,0.02105626 C,0,1.454802925,-0.8075607371,-0.3469932216 C,0,1.8008699956,0.5266635553,-0.3711052683 C,0,0.9301947317,1.6156783044,-0.0559592361 C,0,-0.3915416808,1.2152007002,0.3074265008 C,0,-0.7457048284,-0.1005499692,0.3566057123 H,0,-1.1871847529,-1.3861707711,-0.5234145318 H,0,2.1798119392,-1.5857732377,-0.5611410381 H,0,2.8214004415,0.7627408268,-0.6621177958 H,0,-0.0334566634,-2.1565768421,0.4566332503 H,0,-1.1635420938,1.9676412976,0.4633175318 N,0,-2.1187630948,-0.6644638258,0.2280731119 H,0,-2.7381885454,-0.0722624624,-0.3118541525 H,0,-2.5717072668,-0.9466600933,1.0930588873
T18P3	C,0,-0.064041629,-0.8561103616,-0.0279085722

	C,0,1.3213891601,-0.9409897122,0.022614675 C,0,1.9961676961,0.261763668,0.2005650749 C,0,1.0484012681,1.2275185454,0.0457853121 C,0,-0.2946487111,1.4650651671,-0.0788092932 C,0,-0.9452445775,0.2441399613,0.0474476595 H,0,-0.4818950471,-2.1356383604,-0.1792374644 H,0,1.775293265,-1.9295256316,-0.1015415646 H,0,3.0413166286,0.4335378545,0.42316947 H,0,-0.4168283509,-3.0536210589,-0.2472886231 H,0,-0.7250453235,2.4422319484,-0.2778963803 N,0,-2.2999974313,0.0635632572,0.2407084651 H,0,-2.9102081646,0.8244064495,-0.0082485151 H,0,-2.6737617729,-0.8489427267,0.0342257564
T19P15	C,0,-0.9795880683,-1.3897697298,-0.1728173139 C,0,-1.7699535325,-0.2048555157,-0.1095024736 C,0,-1.08524146,0.9841357007,-0.0907249712 C,0,0.2731396196,1.086594428,0.0277837361 C,0,1.0274735077,-0.1238316343,-0.0375694347 C,0,0.3706308346,-1.3565272602,0.0426670102 H,0,-1.5304167223,-2.320882682,-0.2534702785 H,0,-2.8426277539,-0.2804642265,-0.0231920165 H,0,-1.7841777392,2.0222810233,0.083996514 H,0,0.7996602887,2.0312009318,0.0499180141 H,0,-2.033763281,2.2166092335,0.9532882276 N,0,2.3906903378,-0.0525905845,-0.2156850687 H,0,2.8683750026,0.8009828957,0.0209417553 H,0,2.8976909861,-0.90216959,-0.0358037001
T20P11	C,0,-0.0724088187,0.795886786,-1.7322683512 C,0,0.6407877965,0.2382999916,-0.6766489876 C,0,0.2803940323,0.126070242,0.6545982025 C,0,-0.8852721885,0.7519457624,1.0572831956 C,0,-1.6885987007,1.3066975212,0.039750776 C,0,-1.2159329628,1.3881453789,-1.2748296152 H,0,0.3281068274,0.8921323024,-2.7344294792 H,0,1.6969894004,-1.1248347957,-0.9377759002 H,0,0.9130194144,-0.4043992216,1.3513662861 H,0,-1.1936586374,0.742545618,2.0982617952 H,0,1.8010132915,-0.238177576,-0.940702192 N,0,-2.9527051574,1.7837006337,0.3274755874 H,0,-3.4454387415,1.3919453208,1.1128537524 H,0,-3.5234439356,2.0021635862,-0.4737366098
PR1	C,0,-0.7236306838,-1.3961895392,0.4746996686 C,0,0.6877921878,-1.5187409659,0.8562050566 C,0,1.306248335,-0.3485942258,0.8689822204 C,0,1.0360286985,0.844410386,0.3770268267 C,0,-0.1809058581,0.8436672644,-0.4942068629 C,0,-1.0812108752,-0.31297609,-0.2480237256

	H,0,-1.3949070332,-2.2387746541,0.586675352 H,0,1.1785162005,-2.4810609782,0.7833959792 H,0,1.3727771912,1.795927752,0.7635046925 H,0,-2.0559995214,-0.2701733817,-0.7181590761 N,0,-0.4855920762,1.8827756128,-1.1777084014 H,0,-1.4565980051,1.8507340298,-1.4909883601
PR2	C,0,2.8296286142,-1.2198145889,-0.2020948211 C,0,4.1920002502,-0.8934817237,-0.0723415825 C,0,4.3146452153,0.4684079101,0.0833306536 C,0,3.9375092387,1.7526711676,0.1959513927 C,0,2.8137026117,1.033588736,0.040303675 C,0,2.0159155319,-0.0740757348,-0.1347226158 H,0,2.453715777,-2.2284029961,-0.3371551139 H,0,5.0088259599,-1.5982884548,-0.0918507205 H,0,4.3125318975,2.7588711922,0.3306918567 H,0,0.9394271116,-0.0659539094,-0.208506705
PR3	C,0,-1.1356455077,0.5641228105,0.1019257059 C,0,-2.1380160768,-0.3365400206,0.0706991439 C,0,-0.9588290172,-0.9848621049,-0.0047624514 C,0,0.3893024652,-1.2191991078,-0.0564615546 C,0,1.0627886891,0.033722716,0.0063518274 C,0,0.1241019944,1.100317385,0.1006936734 H,0,-3.210604935,-0.4604875215,0.0923092861 H,0,0.8741091221,-2.1808510137,-0.1356419891 H,0,0.3791058635,2.1480785469,0.1580201109 N,0,2.4164724387,0.1926309872,-0.0559305011 H,0,3.007833994,-0.6066571677,0.0882814843 H,0,2.8152469696,1.0779744908,0.2019722643
PR4	C,0,1.0410785751,1.1435595221,-0.0284365311 C,0,1.9929169469,0.1541951135,-0.0138617955 C,0,1.3174101758,-1.084111578,0.0073160183 C,0,-0.0753981167,-1.192309989,0.0100980779 C,0,-0.9296788308,-0.0620928914,-0.0081162986 C,0,-0.1989224922,1.12258577,-0.0254885693 H,0,3.0662425409,0.2498134551,-0.0174175495 H,0,1.9087593052,-1.9922327901,0.0215980598 H,0,-0.521492121,-2.1802649832,0.0309386964 N,0,-2.3062824185,-0.1559737287,0.0450427736 H,0,-2.8193202948,0.6534222027,-0.2615330573 H,0,-2.7154082698,-1.0304861029,-0.2401308245
PR5	C,0,2.6720385271,-0.5314829567,-0.0268832156 C,0,4.0390774335,-0.3214843991,-0.2529171048 C,0,4.7289321329,0.789021893,0.2681296481 C,0,3.8704886947,1.5849502297,0.9966653193 C,0,2.6601547885,1.3990240111,1.1967887239 C,0,1.8883642043,0.3526662304,0.7378051003 H,0,2.1980891647,-1.406100603,-0.4554589233

	H,0,5.7822945776,0.9524445863,0.0949785401 H,0,0.8348514154,0.1924399345,0.9130165743 H,0,4.5879129391,-1.0389862924,-0.8506058059
PR6	C,0,-1.1668731815,1.1606060244,-0.0768348995 C,0,-0.0131924095,1.1127243713,-0.8051623707 C,0,0.8504001739,2.2151763017,-0.6795896731 C,0,0.314361638,3.5051332925,-0.502664159 C,0,-0.8296878464,3.5977622584,0.2346542036 C,0,-1.6014223016,2.4020419238,0.5496670513 H,0,-1.7499861932,0.2741899461,0.138289629 H,0,0.3192459298,0.1878846342,-1.2611513051 H,0,0.8885660426,4.3876960525,-0.7590708318 H,0,-1.1551023994,4.5422302302,0.6567593327 N,0,-2.6515898545,2.3744170948,1.3055859308 H,0,-2.8629868182,3.3055222301,1.6677011919
PR7	C,0,-0.2674214085,1.1904913679,0.0063540535 C,0,1.2111377485,1.1904276056,-0.003621441 C,0,1.8214902298,-0.0000157843,-0.0076445664 C,0,1.2110841051,-1.1904316021,-0.0036211125 C,0,-0.2674742698,-1.1904284345,0.0063543252 C,0,-0.8778223935,0.0000444164,0.0103859824 H,0,-0.7204435233,2.1706081646,0.0094072717 H,0,1.6641981021,2.1705252119,-0.0066634315 H,0,1.6641009016,-2.1705492739,-0.0066628968 H,0,-0.720540492,-2.1705246717,0.0094078154
PR8	C,0,-0.6616730985,-0.4093597935,1.3872856736 C,0,-0.5401835121,1.033708136,1.3869038127 C,0,-0.5262306441,1.0921163951,-0.0003927053 C,0,-0.5213145045,1.0305270519,-1.3875800762 C,0,-0.6425184507,-0.4120384534,-1.3866982185 C,0,-0.6573121594,-0.46999552,0.0006336472 H,0,-0.7294861065,-1.1507766225,2.1756182985 H,0,-0.4826708459,1.7770288403,2.1743005064 H,0,-0.4534064188,1.7721454521,-2.1757268518 H,0,-0.6993452789,-1.155114485,-2.1743440949
PR9	C,0,-2.0715946396,0.0344807708,0.1945360644 C,0,-0.6267236103,0.2149536903,0.1871279939 C,0,-0.1400168773,1.4774438247,0.097333936 C,0,-1.0165713793,2.5785981315,-0.1178448836 C,0,-2.3818343729,2.4021663193,-0.3549256534 C,0,-2.8873180553,1.2195312625,0.1280502392 H,0,0.0007728295,-0.6644954558,0.12152113 H,0,0.9258857482,1.6641789837,0.1113539077 H,0,-0.6219485847,3.5854140804,-0.0294255036 H,0,-3.0095071464,3.2484586547,-0.6073613437 N,0,-2.5779367676,-1.1612721146,0.1306273846 H,0,-3.5976287543,-1.0915195674,0.1400501985

PR10	C,0,0.9670923503,1.2937380232,-0.875514467 C,0,2.3261463895,1.3210790169,-0.5387839987 C,0,2.5078023821,1.1379741881,0.8181228665 C,0,1.6104268402,0.9824100949,1.6590842967 C,0,0.252205495,0.9418648046,1.4541827326 C,0,-0.058436232,1.1107096402,0.0819767138 H,0,0.6864362982,1.4101857107,-1.9157310434 H,0,-0.519376927,0.8032178961,2.1992785984 H,0,3.0967065124,1.4643089342,-1.282372759 N,0,-1.3895070776,1.0407206846,-0.3383259653 H,0,-1.6048346847,1.5311187291,-1.1915330761 H,0,-2.0778486165,1.2153599574,0.3765951714
PR11	C,0,-0.1174821904,0.0363015566,-0.2230097129 C,0,1.0512000493,0.0684689028,0.5479139518 C,0,1.3345493733,1.3189195326,1.0192942124 C,0,1.0409025504,2.6235827381,1.1201668203 C,0,-0.0035707868,2.2738414661,0.3458774224 C,0,-0.7088847008,1.3075046804,-0.3343603972 H,0,-0.5249284473,-0.8624478288,-0.6766048967 H,0,1.6626816834,-0.7975332717,0.7572762075 H,0,-2.06758059,0.97749141,-1.8190788524 H,0,1.4340983993,3.5148527522,1.5889951107 N,0,-1.9262816723,1.552081588,-1.001257872 H,0,-2.069812348,2.5248662938,-1.224859544
PR12	C,0,-0.7476544234,-0.7892602722,-1.4224051956 C,0,0.567064111,-0.8265421214,-0.9188949722 C,0,0.7979833424,0.2237599807,-0.0096536313 C,0,-0.3664298892,0.9624604602,0.0912877806 C,0,-1.6322223977,1.3792088792,-0.0946381041 C,0,-1.3927056949,0.2897519119,-0.8469615124 H,0,-1.1747059046,-1.481951456,-2.1301592605 H,0,1.3059676408,-1.5692135411,-1.1946644059 H,0,1.7201743624,0.4155528534,0.5155847821 N,0,-2.5746583283,2.2780544908,0.2924750252 H,0,-2.2450008656,3.1225895245,0.730817537 H,0,-3.3784002629,2.38054102,-0.3054865929
PR15	C,0,1.8485924324,-0.6976491662,0.6568264094 C,0,0.8883321228,-0.5342638688,1.5642448859 C,0,0.2948495275,0.8241835722,1.7879839602 C,0,0.8794365719,1.800925626,1.1027241737 C,0,1.8896407526,1.6981499976,0.2413648309 C,0,2.4281526209,0.3381603462,-0.0225862267 H,0,2.55392603,2.5053385655,-0.0428900297 H,0,0.2944481498,-1.329858072,1.9965275394 H,0,-0.6847363972,0.8238940544,2.2425048881 N,0,3.5611225523,0.2470401177,-0.7852924538 H,0,4.1633740938,-0.5432318273,-0.627566617

	H,0,4.0125105333,1.0930012448,-1.0882366903
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**Table S3.** Gibbs free energies ( $\Delta G$ ) in kcal/mol using CCSD(T)//B3LYP/6-311++G(3df,2p) and Entropies ( $\Delta S$ ) in cal/mol.K using B3LYP/6-311++G(3df,2p) of the  $C_6H_5 + NH_2$  reaction at 298.15 K.

Channels	$\Delta G$ (kcal/mol)	$\Delta S$ (cal/mol.K)
$C_6H_5 + NH_2 \rightarrow PR1$	-3.42	-9.36
$C_6H_5 + NH_2 \rightarrow PR2$	-11.15	-1.41
$C_6H_5 + NH_2 \rightarrow PR3$	-3.29	-8.55
$C_6H_5 + NH_2 \rightarrow PR4$	-13.61	-8.73
$C_6H_5 + NH_2 \rightarrow PR5$	-25.01	-1.80
$C_6H_5 + NH_2 \rightarrow PR6$	8.14	-9.65
$C_6H_5 + NH_2 \rightarrow PR7$	2.84	0.86
$C_6H_5 + NH_2 \rightarrow PR8$	32.14	0.82
$C_6H_5 + NH_2 \rightarrow PR9$	7.53	-9.13
$C_6H_5 + NH_2 \rightarrow PR10$	-10.34	-8.33
$C_6H_5 + NH_2 \rightarrow PR11$	4.87	-5.91
$C_6H_5 + NH_2 \rightarrow PR12$	-4.50	-8.36
$C_6H_5 + NH_2 \rightarrow PR15$	21.13	-7.52

**Table S4.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the  $\text{C}_6\text{H}_5 + \text{NH}_2 \rightarrow \text{C}_6\text{H}_5\text{NH}_2$  process in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively.  $K_{\text{eq}}$  ( $\text{cm}^3 \text{ molecule}^{-1}$ ).

T (K)	1 Torr $k_{01}$	10 Torr $k_{02}$	100 Torr $k_{03}$	760 Torr $k_{04}$	7,600 Torr $k_{05}$	76,000 Torr, $k_{06}$	High-P $K_{\text{eq}}$
300	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.18 \times 10^{48}$
400	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.44 \times 10^{29}$
500	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$6.77 \times 10^{17}$
600	$1.58 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.98 \times 10^{10}$
700	$1.55 \times 10^{-9}$	$1.62 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$8.52 \times 10^4$
800	$1.38 \times 10^{-9}$	$1.58 \times 10^{-9}$	$1.65 \times 10^{-9}$	$1.66 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.67 \times 10^{-9}$	$8.34 \times 10^0$
900	$1.07 \times 10^{-9}$	$1.43 \times 10^{-9}$	$1.62 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.68 \times 10^{-9}$	$6.52 \times 10^{-3}$
1000	$7.28 \times 10^{-10}$	$1.17 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.69 \times 10^{-9}$	$2.19 \times 10^{-5}$
1100	$4.33 \times 10^{-10}$	$8.51 \times 10^{-10}$	$1.29 \times 10^{-9}$	$1.55 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.69 \times 10^{-9}$	$2.11 \times 10^{-7}$
1200	$1.65 \times 10^{-10}$	$5.05 \times 10^{-10}$	$9.91 \times 10^{-10}$	$1.37 \times 10^{-9}$	$1.61 \times 10^{-9}$	$1.68 \times 10^{-9}$	$4.49 \times 10^{-9}$
1300	$4.63 \times 10^{-12}$	$4.20 \times 10^{-11}$	$2.89 \times 10^{-10}$	$8.68 \times 10^{-10}$	$1.44 \times 10^{-9}$	$1.65 \times 10^{-9}$	$1.75 \times 10^{-10}$
1400	$7.02 \times 10^{-14}$	$7.01 \times 10^{-13}$	$6.93 \times 10^{-12}$	$5.04 \times 10^{-11}$	$3.81 \times 10^{-10}$	$1.22 \times 10^{-9}$	$1.11 \times 10^{-11}$
1500	$1.57 \times 10^{-15}$	$1.57 \times 10^{-14}$	$1.57 \times 10^{-13}$	$1.19 \times 10^{-12}$	$1.18 \times 10^{-11}$	$1.11 \times 10^{-10}$	$1.02 \times 10^{-12}$
1600	$5.00 \times 10^{-17}$	$5.00 \times 10^{-16}$	$5.00 \times 10^{-15}$	$3.80 \times 10^{-14}$	$3.80 \times 10^{-13}$	$3.79 \times 10^{-12}$	$1.28 \times 10^{-13}$
1700	$2.13 \times 10^{-18}$	$2.13 \times 10^{-17}$	$2.13 \times 10^{-16}$	$1.62 \times 10^{-15}$	$1.62 \times 10^{-14}$	$1.62 \times 10^{-13}$	$2.07 \times 10^{-14}$
1800	$1.17 \times 10^{-19}$	$1.17 \times 10^{-18}$	$1.17 \times 10^{-17}$	$8.90 \times 10^{-17}$	$8.90 \times 10^{-16}$	$8.90 \times 10^{-15}$	$4.13 \times 10^{-15}$
1900	$7.97 \times 10^{-21}$	$7.97 \times 10^{-20}$	$7.97 \times 10^{-19}$	$6.06 \times 10^{-18}$	$6.06 \times 10^{-17}$	$6.06 \times 10^{-16}$	$9.87 \times 10^{-16}$
2000	$6.54 \times 10^{-22}$	$6.54 \times 10^{-21}$	$6.54 \times 10^{-20}$	$4.97 \times 10^{-19}$	$4.97 \times 10^{-18}$	$4.97 \times 10^{-17}$	$2.74 \times 10^{-16}$

**Table S5.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the decomposition process,  $\text{C}_6\text{H}_5\text{NH}_2 \rightarrow \text{C}_6\text{H}_5 + \text{NH}_2$ , in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively.

T (K)	1 Torr $k_{-01}$	10 Torr $k_{-02}$	100 Torr $k_{-03}$	760 Torr $k_{-04}$	7,600 Torr $k_{-05}$	76,000 Torr, $k_{-06}$	High-P $k^\infty(T)$
300	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$	$1.17 \times 10^{-57}$
400	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$	$1.02 \times 10^{-38}$
500	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$	$2.28 \times 10^{-27}$
600	$8.01 \times 10^{-20}$	$8.08 \times 10^{-20}$	$8.09 \times 10^{-20}$	$8.09 \times 10^{-20}$	$8.09 \times 10^{-20}$	$8.09 \times 10^{-20}$	$8.09 \times 10^{-20}$
700	$1.82 \times 10^{-14}$	$1.90 \times 10^{-14}$	$1.92 \times 10^{-14}$	$1.92 \times 10^{-14}$	$1.92 \times 10^{-14}$	$1.92 \times 10^{-14}$	$1.92 \times 10^{-14}$
800	$1.65 \times 10^{-10}$	$1.90 \times 10^{-10}$	$1.98 \times 10^{-10}$	$2.00 \times 10^{-10}$	$2.00 \times 10^{-10}$	$2.00 \times 10^{-10}$	$2.00 \times 10^{-10}$
900	$1.65 \times 10^{-7}$	$2.20 \times 10^{-7}$	$2.48 \times 10^{-7}$	$2.56 \times 10^{-7}$	$2.58 \times 10^{-7}$	$2.58 \times 10^{-7}$	$2.58 \times 10^{-7}$
1000	$3.33 \times 10^{-5}$	$5.35 \times 10^{-5}$	$6.87 \times 10^{-5}$	$7.50 \times 10^{-5}$	$7.71 \times 10^{-5}$	$7.74 \times 10^{-5}$	$7.75 \times 10^{-5}$
1100	$2.05 \times 10^{-3}$	$4.03 \times 10^{-3}$	$6.11 \times 10^{-3}$	$7.34 \times 10^{-3}$	$7.91 \times 10^{-3}$	$8.03 \times 10^{-3}$	$8.05 \times 10^{-3}$
1200	$3.67 \times 10^{-2}$	$1.12 \times 10^{-1}$	$2.21 \times 10^{-1}$	$3.06 \times 10^{-1}$	$3.59 \times 10^{-1}$	$3.75 \times 10^{-1}$	$3.78 \times 10^{-1}$
1300	$2.64 \times 10^{-2}$	$2.40 \times 10^{-1}$	$1.64 \times 10^0$	$4.94 \times 10^0$	$8.20 \times 10^0$	$9.37 \times 10^0$	$9.65 \times 10^0$
1400	$6.36 \times 10^{-3}$	$6.34 \times 10^{-2}$	$6.27 \times 10^{-1}$	$4.56 \times 10^0$	$3.45 \times 10^1$	$1.11 \times 10^2$	$1.52 \times 10^2$
1500	$1.54 \times 10^{-3}$	$1.54 \times 10^{-2}$	$1.54 \times 10^{-1}$	$1.17 \times 10^0$	$1.16 \times 10^1$	$1.09 \times 10^2$	$1.64 \times 10^3$
1600	$3.91 \times 10^{-4}$	$3.91 \times 10^{-3}$	$3.91 \times 10^{-2}$	$2.97 \times 10^{-1}$	$2.97 \times 10^0$	$2.96 \times 10^1$	$1.30 \times 10^4$
1700	$1.03 \times 10^{-4}$	$1.03 \times 10^{-3}$	$1.03 \times 10^{-2}$	$7.84 \times 10^{-2}$	$7.84 \times 10^{-1}$	$7.84 \times 10^0$	$7.93 \times 10^4$
1800	$2.83 \times 10^{-5}$	$2.83 \times 10^{-4}$	$2.83 \times 10^{-3}$	$2.15 \times 10^{-2}$	$2.15 \times 10^{-1}$	$2.15 \times 10^0$	$3.91 \times 10^5$
1900	$8.08 \times 10^{-6}$	$8.08 \times 10^{-5}$	$8.08 \times 10^{-4}$	$6.14 \times 10^{-3}$	$6.14 \times 10^{-2}$	$6.14 \times 10^{-1}$	$1.60 \times 10^6$
2000	$2.39 \times 10^{-6}$	$2.39 \times 10^{-5}$	$2.39 \times 10^{-4}$	$1.82 \times 10^{-3}$	$1.82 \times 10^{-2}$	$1.82 \times 10^{-1}$	$5.57 \times 10^6$

**Table S6.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the  $\text{C}_6\text{H}_5 + \text{NH}_2 \rightarrow \text{PR5}$  reaction in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively.

T (K)	1 Torr $k_1$	10 Torr $k_2$	100 Torr $k_3$	760 Torr $k_4$	7,600 Torr $k_5$	76,000 Torr $k_6$	High-P $k^\infty(T)$
300	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$
400	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$
500	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.55 \times 10^{-9}$
600	$1.58 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$
700	$1.56 \times 10^{-9}$	$1.62 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$
800	$1.41 \times 10^{-9}$	$1.58 \times 10^{-9}$	$1.65 \times 10^{-9}$	$1.66 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.67 \times 10^{-9}$
900	$1.16 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.62 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.68 \times 10^{-9}$
1000	$8.61 \times 10^{-10}$	$1.21 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.70 \times 10^{-9}$
1100	$5.90 \times 10^{-10}$	$9.06 \times 10^{-10}$	$1.30 \times 10^{-9}$	$1.55 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.70 \times 10^{-9}$
1200	$3.71 \times 10^{-10}$	$5.91 \times 10^{-10}$	$1.01 \times 10^{-9}$	$1.38 \times 10^{-9}$	$1.61 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.70 \times 10^{-9}$
1300	$2.34 \times 10^{-10}$	$2.93 \times 10^{-10}$	$4.61 \times 10^{-10}$	$9.09 \times 10^{-10}$	$1.45 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.69 \times 10^{-9}$
1400	$1.53 \times 10^{-10}$	$1.76 \times 10^{-10}$	$2.06 \times 10^{-10}$	$2.52 \times 10^{-10}$	$5.08 \times 10^{-10}$	$1.24 \times 10^{-9}$	$1.69 \times 10^{-9}$
1500	$1.03 \times 10^{-10}$	$1.13 \times 10^{-10}$	$1.25 \times 10^{-10}$	$1.33 \times 10^{-10}$	$1.48 \times 10^{-10}$	$2.33 \times 10^{-10}$	$1.67 \times 10^{-9}$
1600	$7.07 \times 10^{-11}$	$7.54 \times 10^{-11}$	$8.06 \times 10^{-11}$	$8.41 \times 10^{-11}$	$8.71 \times 10^{-11}$	$9.16 \times 10^{-11}$	$1.66 \times 10^{-9}$
1700	$5.01 \times 10^{-11}$	$5.23 \times 10^{-11}$	$5.46 \times 10^{-11}$	$5.63 \times 10^{-11}$	$5.76 \times 10^{-11}$	$5.85 \times 10^{-11}$	$1.64 \times 10^{-9}$
1800	$3.66 \times 10^{-11}$	$3.76 \times 10^{-11}$	$3.86 \times 10^{-11}$	$3.94 \times 10^{-11}$	$4.01 \times 10^{-11}$	$4.05 \times 10^{-11}$	$1.62 \times 10^{-9}$
1900	$2.74 \times 10^{-11}$	$2.79 \times 10^{-11}$	$2.84 \times 10^{-11}$	$2.87 \times 10^{-11}$	$2.90 \times 10^{-11}$	$2.93 \times 10^{-11}$	$1.58 \times 10^{-9}$
2000	$2.10 \times 10^{-11}$	$2.12 \times 10^{-11}$	$2.15 \times 10^{-11}$	$2.16 \times 10^{-11}$	$2.18 \times 10^{-11}$	$2.19 \times 10^{-11}$	$1.52 \times 10^{-9}$

**Table S7.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the  $\text{C}_6\text{H}_5 + \text{NH}_2 \rightarrow \text{C}_6\text{H}_5\text{NH}_2$  reaction in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively. In which the error margins of energy about -2 kcal/mol.

T (K)	1 Torr $k_1$	10 Torr $k_2$	100 Torr $k_3$	760 Torr $k_4$	7,600 Torr $k_5$	76,000 Torr $k_6$	High-P $k^\infty(T)$
300	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$	$1.37 \times 10^{-9}$
400	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.47 \times 10^{-9}$
500	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.55 \times 10^{-9}$
600	$1.59 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$
700	$1.57 \times 10^{-9}$	$1.63 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$	$1.64 \times 10^{-9}$
800	$1.42 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.65 \times 10^{-9}$	$1.66 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.67 \times 10^{-9}$
900	$1.14 \times 10^{-9}$	$1.47 \times 10^{-9}$	$1.63 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.68 \times 10^{-9}$	$1.68 \times 10^{-9}$
1000	$7.97 \times 10^{-10}$	$1.23 \times 10^{-9}$	$1.53 \times 10^{-9}$	$1.65 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.70 \times 10^{-9}$
1100	$4.92 \times 10^{-10}$	$9.22 \times 10^{-10}$	$1.34 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.67 \times 10^{-9}$	$1.70 \times 10^{-9}$	$1.70 \times 10^{-9}$
1200	$2.68 \times 10^{-10}$	$6.17 \times 10^{-10}$	$1.08 \times 10^{-9}$	$1.42 \times 10^{-9}$	$1.63 \times 10^{-9}$	$1.69 \times 10^{-9}$	$1.70 \times 10^{-9}$
1300	$7.20 \times 10^{-11}$	$3.01 \times 10^{-10}$	$7.49 \times 10^{-10}$	$1.19 \times 10^{-9}$	$1.53 \times 10^{-9}$	$1.66 \times 10^{-9}$	$1.69 \times 10^{-9}$
1400	$2.12 \times 10^{-12}$	$1.99 \times 10^{-11}$	$1.55 \times 10^{-10}$	$6.00 \times 10^{-10}$	$1.27 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.69 \times 10^{-9}$
1500	$4.91 \times 10^{-14}$	$4.90 \times 10^{-14}$	$4.85 \times 10^{-12}$	$3.54 \times 10^{-11}$	$2.83 \times 10^{-10}$	$1.08 \times 10^{-9}$	$1.67 \times 10^{-9}$
1600	$1.57 \times 10^{-15}$	$1.57 \times 10^{-14}$	$1.57 \times 10^{-13}$	$1.19 \times 10^{-12}$	$1.18 \times 10^{-11}$	$1.10 \times 10^{-10}$	$1.66 \times 10^{-9}$
1700	$6.71 \times 10^{-17}$	$6.71 \times 10^{-16}$	$6.71 \times 10^{-15}$	$5.10 \times 10^{-14}$	$5.10 \times 10^{-13}$	$5.08 \times 10^{-12}$	$1.64 \times 10^{-9}$
1800	$3.69 \times 10^{-18}$	$3.69 \times 10^{-17}$	$3.69 \times 10^{-16}$	$2.80 \times 10^{-15}$	$2.80 \times 10^{-14}$	$2.80 \times 10^{-13}$	$1.62 \times 10^{-9}$
1900	$2.52 \times 10^{-19}$	$2.52 \times 10^{-18}$	$2.52 \times 10^{-17}$	$1.91 \times 10^{-16}$	$1.91 \times 10^{-15}$	$1.91 \times 10^{-14}$	$1.58 \times 10^{-9}$
2000	$2.07 \times 10^{-20}$	$2.07 \times 10^{-19}$	$2.07 \times 10^{-18}$	$1.57 \times 10^{-17}$	$1.57 \times 10^{-16}$	$1.57 \times 10^{-15}$	$1.52 \times 10^{-9}$

**Table S8.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the decomposition process,  $\text{C}_6\text{H}_5\text{NH}_2 \rightarrow \text{C}_6\text{H}_5 + \text{NH}_2$ , in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively. In which the error margins of energy about -2 kcal/mol.

T (K)	1 Torr $k_{-01}$	10 Torr $k_{-02}$	100 Torr $k_{-03}$	760 Torr $k_{-04}$	7,600 Torr $k_{-05}$	76,000 Torr, $k_{-06}$	High-P $k^\infty(T)$
300	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$	$4.07 \times 10^{-59}$
400	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$	$8.22 \times 10^{-40}$
500	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$	$3.05 \times 10^{-28}$
600	$1.50 \times 10^{-20}$	$1.51 \times 10^{-20}$	$1.51 \times 10^{-20}$	$1.51 \times 10^{-20}$	$1.51 \times 10^{-20}$	$1.51 \times 10^{-20}$	$1.51 \times 10^{-20}$
700	$4.37 \times 10^{-15}$	$4.53 \times 10^{-15}$	$4.56 \times 10^{-15}$	$4.56 \times 10^{-15}$	$4.56 \times 10^{-15}$	$4.56 \times 10^{-15}$	$4.56 \times 10^{-15}$
800	$4.85 \times 10^{-11}$	$5.45 \times 10^{-11}$	$5.64 \times 10^{-11}$	$5.67 \times 10^{-11}$	$5.68 \times 10^{-11}$	$5.68 \times 10^{-11}$	$5.68 \times 10^{-11}$
900	$5.71 \times 10^{-8}$	$7.38 \times 10^{-8}$	$8.17 \times 10^{-8}$	$8.38 \times 10^{-8}$	$8.43 \times 10^{-8}$	$8.44 \times 10^{-8}$	$8.44 \times 10^{-8}$
1000	$1.33 \times 10^{-5}$	$2.06 \times 10^{-5}$	$2.57 \times 10^{-5}$	$2.76 \times 10^{-5}$	$2.82 \times 10^{-5}$	$2.83 \times 10^{-5}$	$2.83 \times 10^{-5}$
1100	$9.34 \times 10^{-4}$	$1.75 \times 10^{-3}$	$2.55 \times 10^{-3}$	$2.99 \times 10^{-3}$	$3.18 \times 10^{-3}$	$3.22 \times 10^{-3}$	$3.23 \times 10^{-3}$
1200	$2.58 \times 10^{-2}$	$5.94 \times 10^{-2}$	$1.04 \times 10^{-1}$	$1.37 \times 10^{-1}$	$1.57 \times 10^{-1}$	$1.62 \times 10^{-1}$	$1.63 \times 10^{-1}$
1300	$1.89 \times 10^{-1}$	$7.92 \times 10^{-1}$	$1.97 \times 10^0$	$3.12 \times 10^0$	$4.02 \times 10^0$	$4.36 \times 10^0$	$4.45 \times 10^0$
1400	$9.36 \times 10^{-2}$	$8.77 \times 10^{-1}$	$6.84 \times 10^0$	$2.65 \times 10^1$	$5.59 \times 10^1$	$7.02 \times 10^1$	$7.43 \times 10^1$
1500	$2.46 \times 10^{-2}$	$2.46 \times 10^{-1}$	$2.43 \times 10^0$	$1.78 \times 10^1$	$1.42 \times 10^2$	$5.41 \times 10^2$	$8.40 \times 10^2$
1600	$6.53 \times 10^{-3}$	$6.53 \times 10^{-2}$	$6.53 \times 10^{-1}$	$4.95 \times 10^0$	$4.90 \times 10^1$	$4.57 \times 10^2$	$6.92 \times 10^3$
1700	$1.79 \times 10^{-3}$	$1.79 \times 10^{-2}$	$1.79 \times 10^{-1}$	$1.36 \times 10^0$	$1.36 \times 10^1$	$1.36 \times 10^2$	$4.39 \times 10^4$
1800	$5.10 \times 10^{-4}$	$5.10 \times 10^{-3}$	$5.10 \times 10^{-2}$	$3.88 \times 10^{-1}$	$3.88 \times 10^0$	$3.88 \times 10^1$	$2.23 \times 10^5$
1900	$1.50 \times 10^{-4}$	$1.50 \times 10^{-3}$	$1.50 \times 10^{-2}$	$1.14 \times 10^{-1}$	$1.14 \times 10^0$	$1.14 \times 10^1$	$9.42 \times 10^5$
2000	$4.57 \times 10^{-5}$	$4.57 \times 10^{-4}$	$4.57 \times 10^{-3}$	$3.47 \times 10^{-2}$	$3.47 \times 10^{-1}$	$3.47 \times 10^0$	$3.37 \times 10^6$

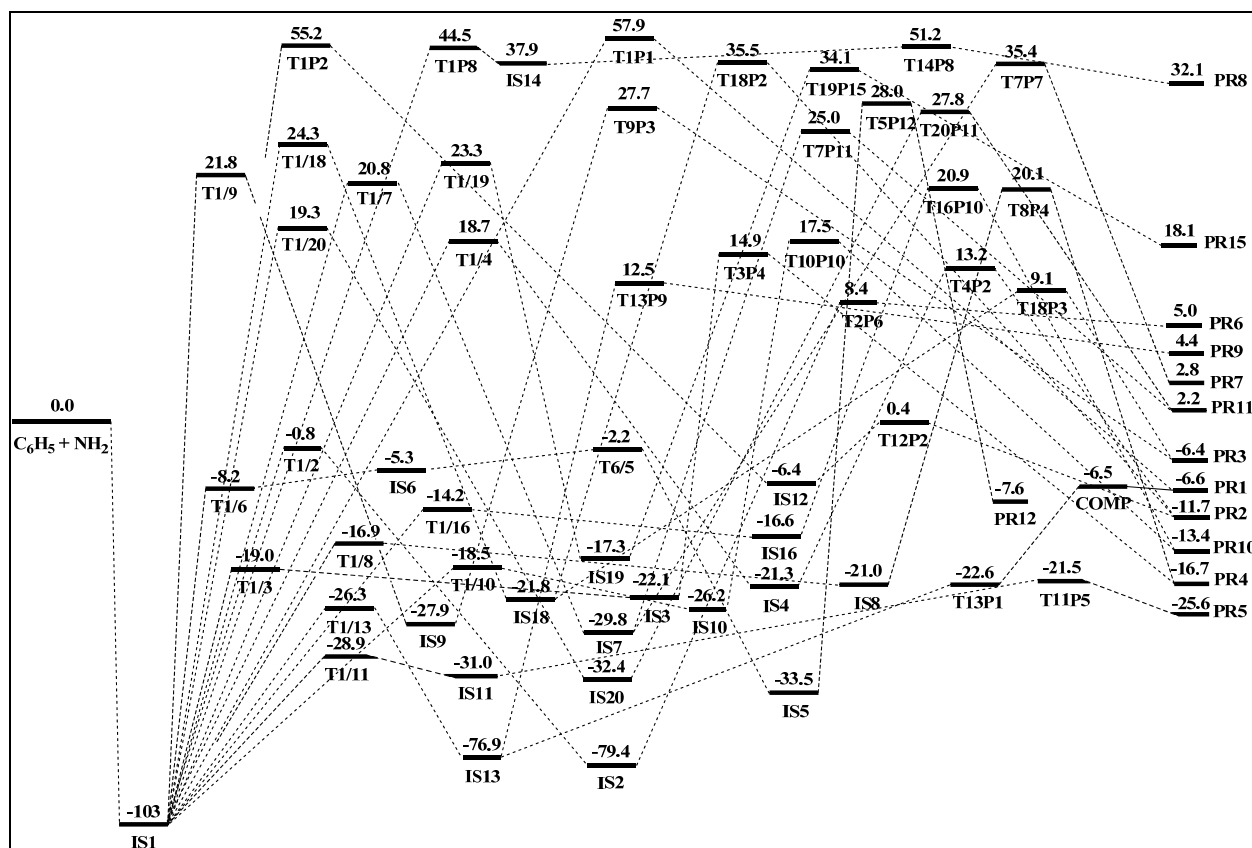
**Table S9.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the  $\text{C}_6\text{H}_5 + \text{NH}_2 \rightarrow \text{C}_6\text{H}_5\text{NH}_2$  reaction in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively. In which the error margins of energy about 2 kcal/mol.

T (K)	1 Torr $k_1$	10 Torr $k_2$	100 Torr $k_3$	760 Torr $k_4$	7,600 Torr $k_5$	76,000 Torr $k_6$	High-P $k^\infty(T)$
300	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$	$1.35 \times 10^{-9}$
400	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.44 \times 10^{-9}$
500	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.50 \times 10^{-9}$
600	$1.52 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.54 \times 10^{-9}$
700	$1.47 \times 10^{-9}$	$1.55 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.57 \times 10^{-9}$
800	$1.28 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.59 \times 10^{-9}$
900	$9.64 \times 10^{-10}$	$1.33 \times 10^{-9}$	$1.53 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.60 \times 10^{-9}$
1000	$6.33 \times 10^{-10}$	$1.06 \times 10^{-9}$	$1.40 \times 10^{-9}$	$1.55 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.61 \times 10^{-9}$	$1.61 \times 10^{-9}$
1100	$3.64 \times 10^{-10}$	$7.46 \times 10^{-10}$	$1.17 \times 10^{-9}$	$1.44 \times 10^{-9}$	$1.57 \times 10^{-9}$	$1.60 \times 10^{-9}$	$1.61 \times 10^{-9}$
1200	$1.07 \times 10^{-10}$	$3.96 \times 10^{-10}$	$8.64 \times 10^{-10}$	$1.25 \times 10^{-9}$	$1.50 \times 10^{-9}$	$1.59 \times 10^{-9}$	$1.60 \times 10^{-9}$
1300	$2.17 \times 10^{-12}$	$2.05 \times 10^{-11}$	$1.64 \times 10^{-10}$	$6.35 \times 10^{-10}$	$1.28 \times 10^{-9}$	$1.54 \times 10^{-9}$	$1.60 \times 10^{-9}$
1400	$3.42 \times 10^{-14}$	$3.42 \times 10^{-13}$	$3.40 \times 10^{-12}$	$2.52 \times 10^{-11}$	$2.14 \times 10^{-10}$	$9.43 \times 10^{-10}$	$1.59 \times 10^{-9}$
1500	$8.04 \times 10^{-16}$	$8.04 \times 10^{-15}$	$8.03 \times 10^{-14}$	$6.10 \times 10^{-13}$	$6.07 \times 10^{-12}$	$5.85 \times 10^{-11}$	$1.57 \times 10^{-9}$
1600	$2.66 \times 10^{-17}$	$2.66 \times 10^{-16}$	$2.66 \times 10^{-15}$	$2.02 \times 10^{-14}$	$2.02 \times 10^{-13}$	$2.02 \times 10^{-12}$	$1.56 \times 10^{-9}$
1700	$1.18 \times 10^{-18}$	$1.18 \times 10^{-17}$	$1.18 \times 10^{-16}$	$8.97 \times 10^{-16}$	$8.97 \times 10^{-15}$	$8.97 \times 10^{-14}$	$1.54 \times 10^{-9}$
1800	$6.70 \times 10^{-20}$	$6.70 \times 10^{-19}$	$6.70 \times 10^{-18}$	$5.09 \times 10^{-17}$	$5.09 \times 10^{-16}$	$5.09 \times 10^{-15}$	$1.52 \times 10^{-9}$
1900	$4.70 \times 10^{-21}$	$4.70 \times 10^{-20}$	$4.70 \times 10^{-19}$	$3.57 \times 10^{-18}$	$3.57 \times 10^{-17}$	$3.57 \times 10^{-16}$	$1.48 \times 10^{-9}$
2000	$3.96 \times 10^{-22}$	$3.96 \times 10^{-21}$	$3.96 \times 10^{-20}$	$3.01 \times 10^{-19}$	$3.01 \times 10^{-18}$	$3.01 \times 10^{-17}$	$1.44 \times 10^{-9}$

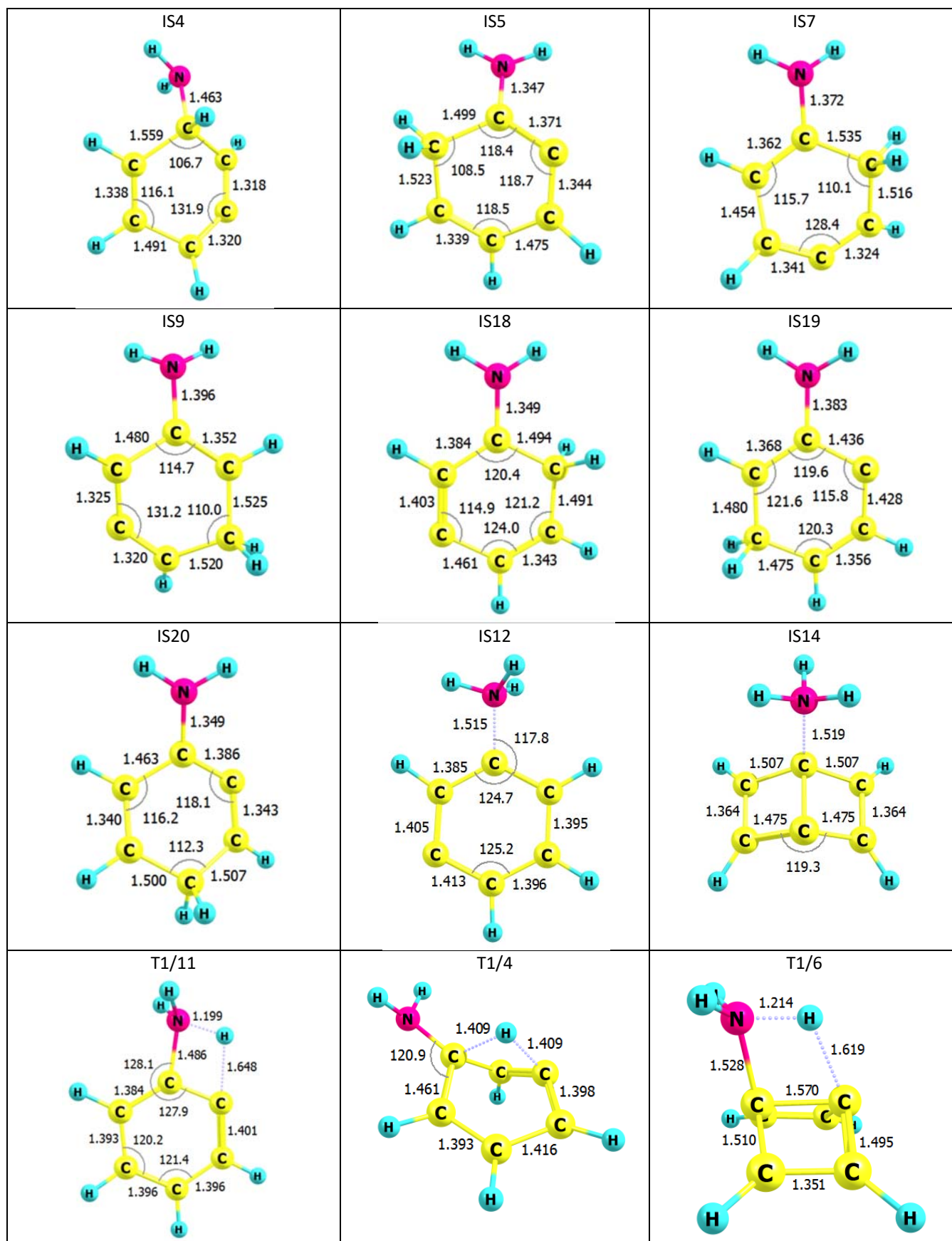
**Table S10.** Predicted rate constants ( $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for the decomposition process,  $\text{C}_6\text{H}_5\text{NH}_2 \rightarrow \text{C}_6\text{H}_5 + \text{NH}_2$ , in the temperature and pressure ranges of 300-2000 K and 1-76,000 Torr, respectively. In which the error margins of energy about 2 kcal/mol.

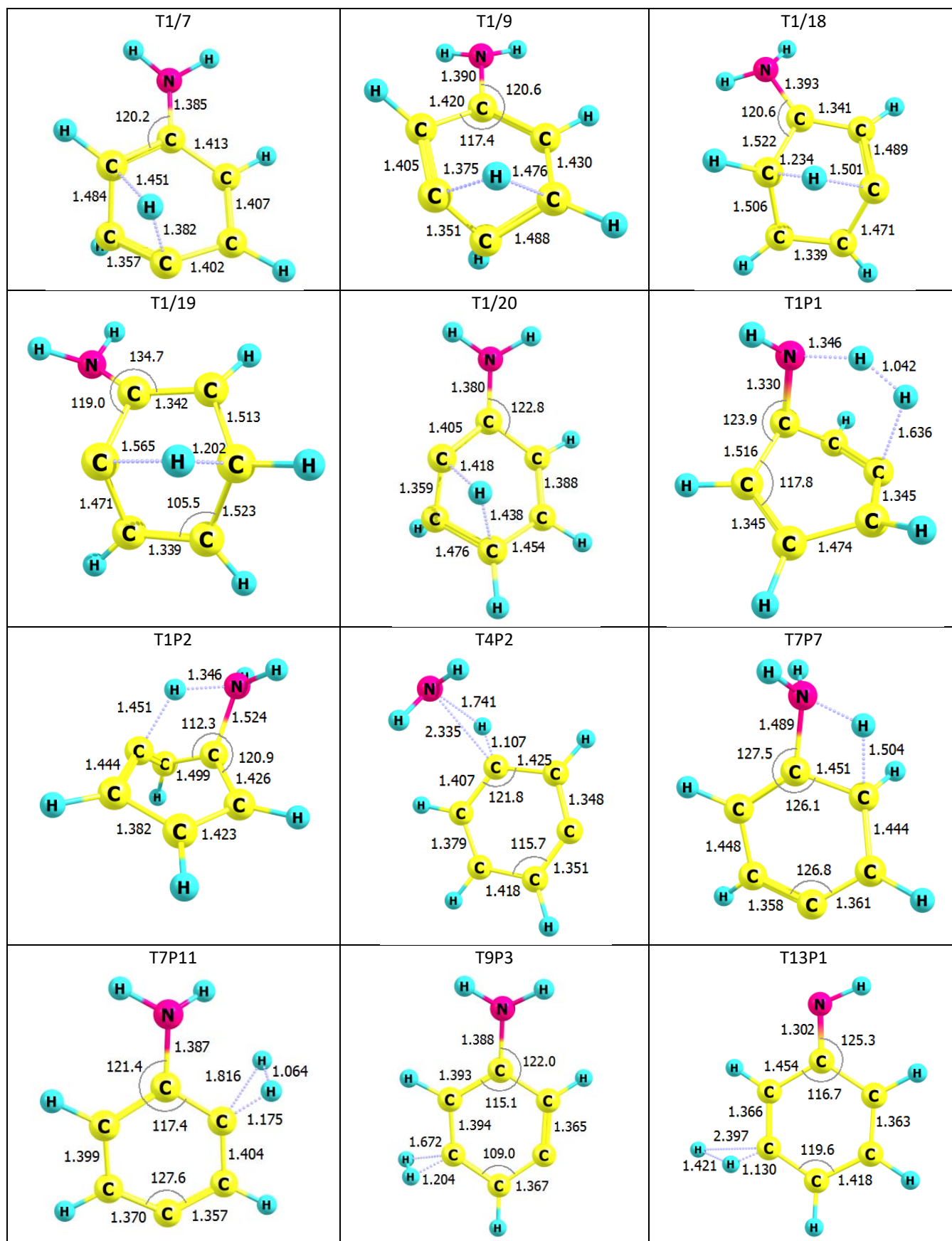
T (K)	1 Torr $k_{-01}$	10 Torr $k_{-02}$	100 Torr $k_{-03}$	760 Torr $k_{-04}$	7,600 Torr $k_{-05}$	76,000 Torr, $k_{-06}$	High-P $k^\infty(T)$
300	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$	$3.30 \times 10^{-56}$
400	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$	$1.23 \times 10^{-37}$
500	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$	$1.66 \times 10^{-26}$
600	$4.12 \times 10^{-19}$	$4.17 \times 10^{-19}$	$4.18 \times 10^{-19}$	$4.18 \times 10^{-19}$	$4.18 \times 10^{-19}$	$4.18 \times 10^{-19}$	$4.18 \times 10^{-19}$
700	$7.26 \times 10^{-14}$	$7.66 \times 10^{-14}$	$7.76 \times 10^{-14}$	$7.77 \times 10^{-14}$	$7.77 \times 10^{-14}$	$7.77 \times 10^{-14}$	$7.77 \times 10^{-14}$
800	$5.38 \times 10^{-10}$	$6.31 \times 10^{-10}$	$6.64 \times 10^{-10}$	$6.71 \times 10^{-10}$	$6.72 \times 10^{-10}$	$6.72 \times 10^{-10}$	$6.72 \times 10^{-10}$
900	$4.52 \times 10^{-07}$	$6.23 \times 10^{-07}$	$7.16 \times 10^{-07}$	$7.44 \times 10^{-07}$	$7.51 \times 10^{-07}$	$7.52 \times 10^{-07}$	$7.52 \times 10^{-07}$
1000	$7.92 \times 10^{-05}$	$1.32 \times 10^{-04}$	$1.75 \times 10^{-04}$	$1.93 \times 10^{-04}$	$2.00 \times 10^{-04}$	$2.01 \times 10^{-04}$	$2.01 \times 10^{-04}$
1100	$4.30 \times 10^{-03}$	$8.83 \times 10^{-03}$	$1.39 \times 10^{-02}$	$1.70 \times 10^{-02}$	$1.86 \times 10^{-02}$	$1.90 \times 10^{-02}$	$1.90 \times 10^{-02}$
1200	$5.49 \times 10^{-02}$	$2.04 \times 10^{-01}$	$4.45 \times 10^{-01}$	$6.44 \times 10^{-01}$	$7.75 \times 10^{-01}$	$8.18 \times 10^{-01}$	$8.27 \times 10^{-01}$
1300	$2.68 \times 10^{-02}$	$2.54 \times 10^{-01}$	$2.02 \times 10^0$	$7.85 \times 10^0$	$1.58 \times 10^1$	$1.90 \times 10^1$	$1.97 \times 10^1$
1400	$6.36 \times 10^{-03}$	$6.35 \times 10^{-02}$	$6.31 \times 10^{-01}$	$4.68 \times 10^0$	$3.98 \times 10^1$	$1.75 \times 10^2$	$2.94 \times 10^2$
1500	$1.54 \times 10^{-03}$	$1.54 \times 10^{-02}$	$1.54 \times 10^{-01}$	$1.17 \times 10^0$	$1.17 \times 10^1$	$1.12 \times 10^2$	$3.02 \times 10^3$
1600	$3.91 \times 10^{-04}$	$3.91 \times 10^{-03}$	$3.91 \times 10^{-02}$	$2.97 \times 10^{-01}$	$2.97 \times 10^0$	$2.96 \times 10^1$	$2.29 \times 10^4$
1700	$1.03 \times 10^{-04}$	$1.03 \times 10^{-03}$	$1.03 \times 10^{-02}$	$7.84 \times 10^{-02}$	$7.84 \times 10^{-01}$	$7.84 \times 10^0$	$1.35 \times 10^5$
1800	$2.83 \times 10^{-05}$	$2.83 \times 10^{-04}$	$2.83 \times 10^{-03}$	$2.15 \times 10^{-02}$	$2.15 \times 10^{-01}$	$2.15 \times 10^0$	$6.42 \times 10^5$
1900	$8.08 \times 10^{-06}$	$8.08 \times 10^{-05}$	$8.08 \times 10^{-04}$	$6.14 \times 10^{-03}$	$6.14 \times 10^{-02}$	$6.14 \times 10^{-01}$	$2.55 \times 10^6$
2000	$2.39 \times 10^{-06}$	$2.39 \times 10^{-05}$	$2.39 \times 10^{-04}$	$1.82 \times 10^{-03}$	$1.82 \times 10^{-02}$	$1.82 \times 10^{-01}$	$8.68 \times 10^6$

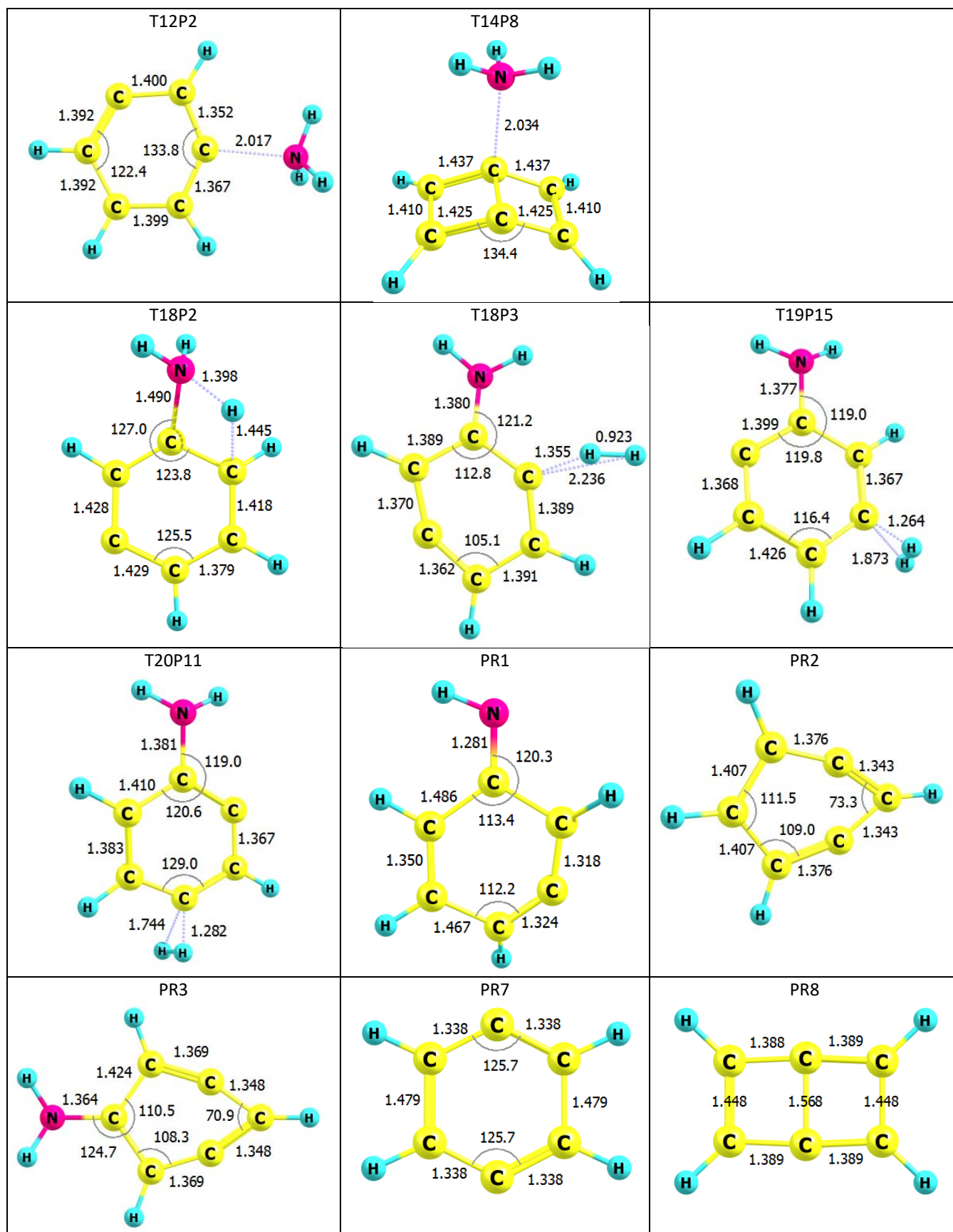


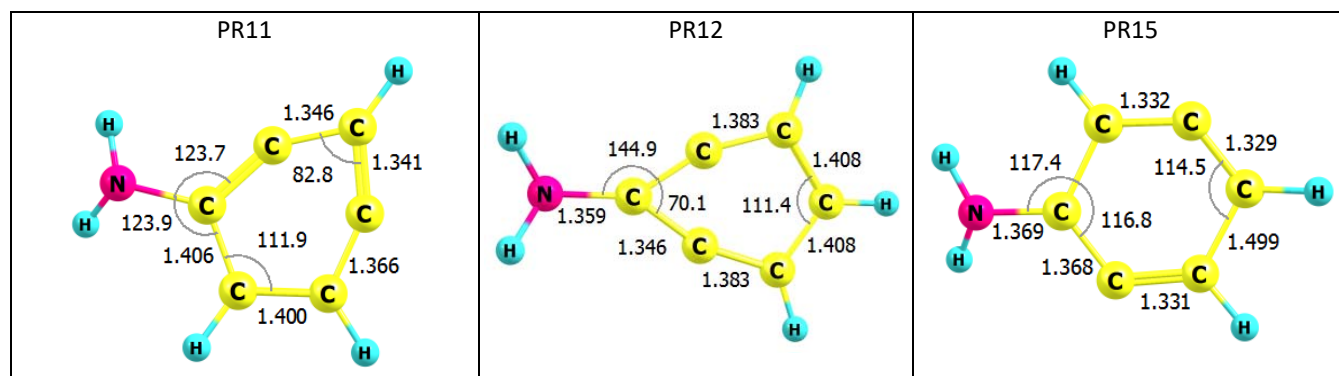


**Figure S1.** Detailed potential energy surface of the  $C_6H_5 + NH_2$  system. Energies are in units of kcal/mol calculated at the B3LYP/6311++G(3df,2p) + ZPVE level.

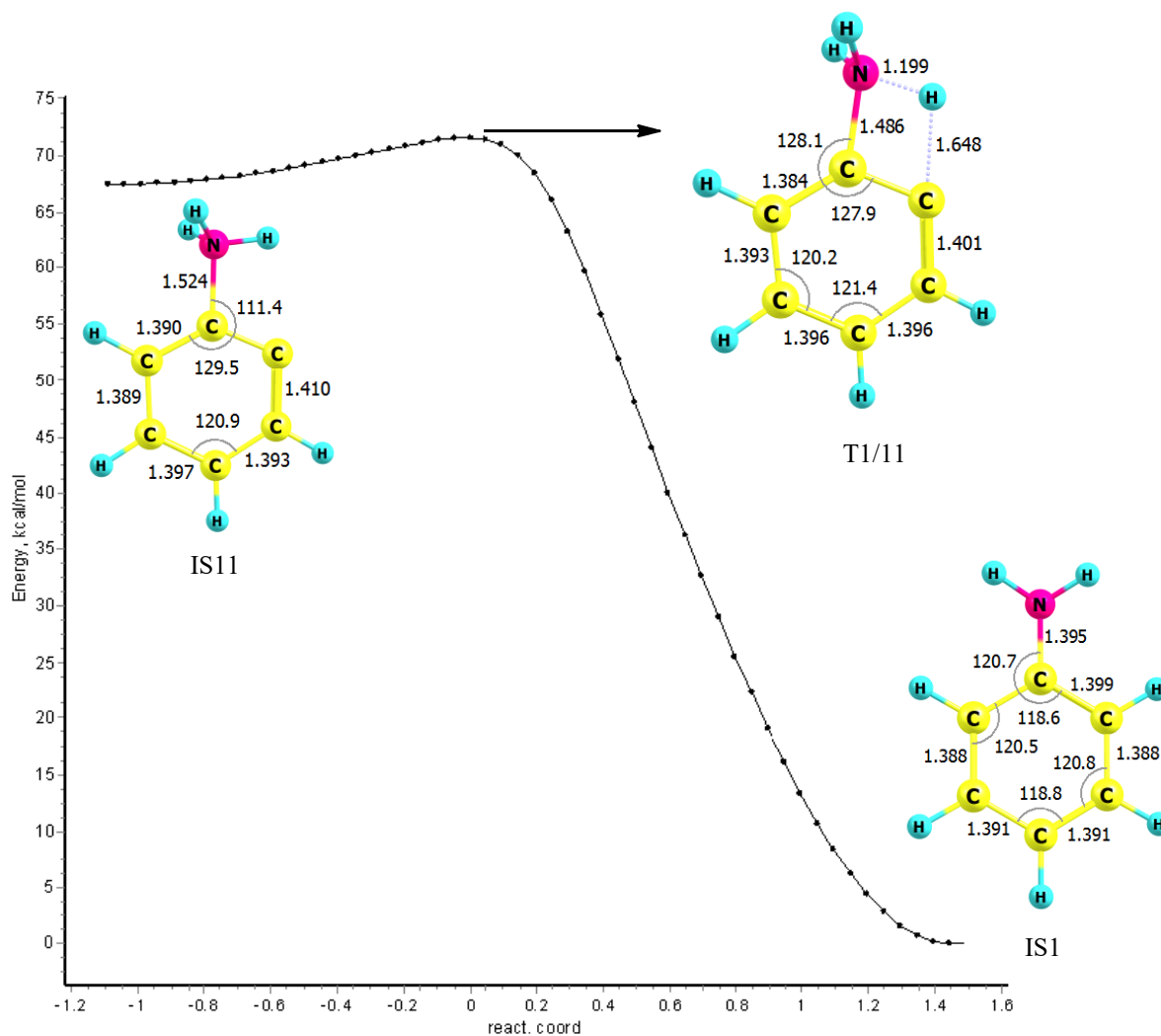








**Figure S2.** Geometries of the reactants, intermediate states, transition states and products optimized at the B3LYP/6-311++G(3df,2p) level.



**Figure S3.** The IRC profile for the transition state T1/11 calculated at the B3LYP/6-311++G(3df,2p) level of theory.